TOWARDS A MACROSTATISTICAL MECANICS*

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ABSTRACT

I discuss the general question of the derivation of the statistical mechanics of macroscopic variables from the quantum structures of many-particle systems, as represented in the thermodynamic limit. I then present a number of strands of such a macrostatistical mechanics, including (a) a derivation of the electrodynamics of superconductors from their order structure and gauge covariance; (b) a hydrodynamics, with transition from deterministic to stochastic flow, of a quantum plasma model; and (c) a non-linear generalisation of Onsager's irreversible thermodynamics.

1. Introduction. The 'miracle' of statistical physics is that the microscopically chaotic dynamics of many-particle systems conspires to generate macroscopic laws of relatively simple structure, such as those of thermodynamics and hydrodynamics. In view of the complexity of the microscopic picture and the simplicity of the macroscopic one, it is natural to seek an approach to the subject, that is centred on macro- observables, with microscopic imput limited to very general principles, e.g. conservation laws, ergodicity, etc. Such an approach would evidently be at the opposite pole from the conventional microscopically based 'many-body theory'.

In fact, there are already important macroscopically-based theories in statistical physics, most notably Onsager's [On] linear irreversible thermodynamics and Landau's [LL, Ch.17]] fluctuating hydrodynamics. However, these theories are essentially heuristic because, apart from questions of rigour, they lack the structures needed for a precise characterisation of their purportedly key ingredient of macroscopicality. Moreover, the same

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thing can be said about all works devised within the traditional framework of the statistical mechanics of strictly finite systems.

On the other hand, the 'revolution' in statistical mechanics, based on the formulation of many-particle systems in the thermodynamic limit [Ru, HHW, He], have provided us with just the framework required for a sharp characterisation of macroscopicality, and even of different levels thereof [Se1, GVV]. My objective here is to discuss the project of extracting a 'macrostatistical mechanics' (MSM) from the quantum structures of many-particle systems, within this framework. In fact, we already have some strands of such a discipline in the works of Hepp and Lieb [HL] on the derivation of the macroscopic dynamics, with non-equibrium phase transition, of a laser mode; of myself [Se1,Ch.4] on the formulation of an extended classical thermodynamics with phase structure; and of the Leuven school [GVV] on macroscopic fluctuation theory.

In this article, I shall bring together further contributions, from three different areas, towards an MSM. The first of these, (§2), consists of a derivation of the electromagnetic properties of superconductors from their order structure and gauge covariance [Se2,3]. The second, (§3), is an extraction of the hydrodynamics, with non-equilibrium phase transition, of a quantum plasma model [Se4]; and the third, (§4), consists of a quantum-statistical derivation of a non-linear generalisation of Onsager's irreversible thermodynamics [Se5]. I shall conclude, in §5, with some further brief comments about the project of a macroscopically-centred statistical mechanics.

2. Macroscopic Quantum Theory of Superconductivity. At the *phenomenological* level, the principal electrodynamic properties of superconductors are their capacity to support persistent electric currents (superconductivity) and their perfect diagmagnetism (Meissner effect). These two properties are intimately related, since the Meissner effect is the mechanism whereby the supercurrents screen the magnetic field they generate from the interior of the body [Lo]. Thus, superconductivity arises from the combination of the Meissner effect with the thermodynamic metastability of the supercurrents and their magnetic fields.

Although it appears to be widely accepted that the microscopic theory of Bardeen-Cooper-Schrieffer [BCS] leads to the electrodynamics of metallic superconductors, the arguments employed both there and in related works [An, Ri] are radically flawed in that (a) they are based on totally uncontrolled approximations, and (b) they violate (exact) gauge covariance of the second kind *at the Hamiltonian level*, and thus do not even admit precise definition of a local current density. As regards ceramic, i.e. high T_c, superconductivity, the microscopic theory is less developed than in the metallic case, and has not yet led to an electrodynamics.

On the other hand, the BCS characterisation of the structure of the superconductive phase by electron pairing, first proposed by Schafroth [Sc], has been amply substantiated by experiments on the Josephson effect [Jo] and the quantisation of trapped magnetic flux in multiply-connected superconductors [DF]. Moreover, Yang [Ya], generalising ideas of O. Penrose [Pe, PO], pointed out that this characterisation is captured by the hypothesis of *off-diagonal long range order* (ODLRO). This is a macroscopic quantum property, representing a well-defined order structure in a gauge covariant way. Furthermore, it is a property also possessed by certain ansätze, e.g. [ZA], for the high T_c superconductive phase of ceramics.

I shall now sketch an approach [Se2,3] I have made to the electrodynamics of superconductors, based on the assumption of ODLRO. This is designed to relate the electromagnetic properties to the order structure of these systems in purely macroscopic quantum terms (cf. eqno. (2.8) below). For brevity, I shall confine myself here to the derivation of the Meissner effect from ODLRO.

The Model. We take the quantum model, Σ, to be an infinitely extended system of electrons, and possibly also of ions or phonons, in a Euclidean space X : lattice systems may be formulated analogously. Points in X will generally be denoted by x, (sometimes by y, a or b) and the Lebesgue measure by dx. It will be assumed that the model enjoys the properties of gauge covariance of the second kind, and that its interactions are translationally invariant.

The electronic part of Σ is formulated in terms of a quantised field $\psi = (\psi_\uparrow, \psi_\downarrow)$, satisfying the canonical anticommutation relations. Thus, in a standard way, the $C^\star-$algebra $\mathcal{F}_{el}$ of the CAR over the Hilbert space $\mathcal{H} := L^2(X, dx)$ is defined by the specifictions that

(1) there are linear maps $\psi_\uparrow, \psi_\downarrow$, from $\mathcal{H}$ into $\mathcal{F}_{el}$ satisfying the CAR

$$[\psi_\alpha(f), \psi_\beta(g)^\star]_+ = \delta_{\alpha,\beta}\langle g, f\rangle_{\mathcal{H}};\ [\psi_\alpha(f), \psi_\beta(g)]_+ = 0 \tag{2.1}$$

(2) $\mathcal{F}_{el}$ is generated by $\{\psi_\alpha(f), \psi_\alpha(f)^\star | f\in\mathcal{H};\ \alpha = \uparrow, \downarrow\}$.

The algebra $\mathcal{F}_{el}$ is then the *field algebra* of the electrons. Space translations and gauge transformations are represented by the homomorphisms $\sigma_0,\ \gamma$ of the additive groups $X,\ C_R^\infty(X)$, respectively, into $Aut(\mathcal{F}_{el})$, defined by the formulae

$$\sigma_0(a)\psi(f) = \psi(f_a)\ \forall a\in X,\ \mathit{with}\ f_a(x) := f(x-a) \tag{2.2}$$

and

$$\gamma(\chi)\psi(\phi) = \psi(\phi\exp(i\chi))\ \forall\chi\in C_R^\infty(X) \tag{2.3}$$

The *global* gauge automorphisms are those for which χ is constant.

Let $\mathcal{K} := \{f_1 \otimes f_2 | f_1, f_2 \in \mathcal{H}\}$. We define the *pair field* Ψ to be the mapping of $\mathcal{K}$ into $\mathcal{F}_{el}$ given by

$$\Psi(F) = \psi_\uparrow(f_1)\psi_\downarrow(f_2)\ for\ F = f_1 \otimes f_2 \tag{2.4}$$

Hence, by (2.2)-(2.4),

$$\sigma_0(a)\Psi(F) = \Psi(F_a),\ with\ F_a(x_1, x_2) = F(x_1 - a, x_2 - a) \tag{2.5}$$

and

$$\gamma(\chi)\Psi(F) = \Psi(g(\chi)F); \tag{2.6}$$

$$with\ (g(\chi)F)(x_1, x_2) := F(x_1, x_2)\exp i(\chi(x_1) + \chi(x_2))$$

In a standard way, we define the *observable algebra* of the electrons to be the subalgebra $\mathcal{A}_{el}$ of $\mathcal{F}_{el}$ that is elementwise invariant under the global gauge automorphisms $\psi \to \psi\exp(i\alpha)$, with α constant. Space translations and gauge transformations of the electronic observables are then given by the restrictions to $\mathcal{A}_{el}$ of the automorphism groups $\sigma_0(X)$ and $\gamma(C_R^\infty(X))$, respectively.

The construction of the $C^\star-$algebra $\mathcal{A}_0$ of the observables of the other species of particles of Σ is effected in a similar way. We take the $C^\star-$algebra of observables of the system to be $\mathcal{A} := \mathcal{A}_{el} \otimes \mathcal{A}_0$ and canonically identify $\mathcal{A}_{el}$ with its subalgebra $\mathcal{A}_{el} \otimes I$. It is assumed that the automorphism groups $\sigma_0(X)$ and $\gamma(C_R^\infty(X))$ extend from $\mathcal{A}_{el}$ to $\mathcal{A}$.

We assume, for simplicity,* that the dynamics of Σ, as given by a canonical limiting form of that of finite versions of the system, corresponds to a one-parameter group $\{\alpha(t) | t \in \mathbf{R}\}$ of automorphisms of $\mathcal{A}$.

An equilibrium state ω at inverse temperature β may then be characterised by the Kubo-Martin-Schwinger (KMS) conditions [HHW], namely that, for arbitrary $A, B \in \mathcal{A}$, there is a function F on $\mathbf{C}$ that is analytic in the interior of the strip $Im(z) \in [0, \hbar\beta]$ and continuous on its boundaries, and satisfies the relations

$$F(t) = \omega(A\alpha(t)B);\ F(t + i\hbar\beta) = \omega((\alpha(t)A)B) \tag{2.7}$$

Off-Diagonal Long Range Order. A state ω is said to possess the property of off-diagonal long-range order (ODLRO) if there is a mapping $\Phi : \mathcal{K} \to \mathbf{C}$, such that

$$\lim_{|y| \to \infty}[\omega(\Psi(F)^\star\Psi(G_y)) - \overline{\Phi(F)}\Phi(G_y)] = 0\ \forall F, G \in \mathcal{K} \tag{2.8}$$

* The more generally valid assumption of a $W^\star-$dynamical system [Se6], employed in §4 of this article, leads to precisely the same results as the present one.

where the bar denotes complex conjugation; and $\Phi(G_y)$ does not tend to zero, for all $G \in \mathcal{K}$ as $y \rightarrow \infty$.

Φ is then termed the *macroscopic wave function* for the state ω.

Note that, although $\Psi(F)$ does not belong to the observable algebra $\mathcal{A}$, the argument of ω in (2.8) does.

Lemma 2.1. *The ODLRO conditions define the macroscopic wave function up to a constant phase factor; i.e., if Φ_1, Φ_2 are two such functions satisfying these conditions, for the same state ω, then $\Phi_2 = \Phi_1 \exp(i\eta)$, where η is a real-valued constant.*

Proof. Assuming that Φ_1, Φ_2 both satisfy the ODLRO conditions with respect to the same state ω, it follows from (2.8) that

$$\lim_{|y| \rightarrow \infty} [\overline{\Phi_1(F)} \Phi_1(G_y) - \overline{\Phi_2(F)} \Phi_2(G_y)] = 0$$

Since this is valid for all $F, G \in \mathcal{K}$, we may replace F by $F'(\in \mathcal{K})$, thereby obtaining

$$\lim_{|y| \rightarrow \infty} [\overline{\Phi_1(F')} \Phi_1(G_y) - \overline{\Phi_2(F')} \Phi_2(G_y)] = 0$$

On multiplying the complex conjugate of the first equation by $\Phi_2(F')$ and that of the second one by $\Phi_2(F)$, and then taking the difference, we see that

$$\lim_{|y| \rightarrow \infty} \overline{\Phi_1(G_y)} [\Phi_1(F) \Phi_2(F')) - \Phi_1(F') \Phi_2(F)] = 0 \tag{2.9}$$

Since, by the above definition of ODLRO, there are elements G of $\mathcal{K}$ for which $\Phi(G_y)$ does not tend to zero, as $|y| \rightarrow \infty$, it follows that the quantity in the square brackets of (2.9) vanishes. Consequently, as $\Phi_{1,2}$ are non-zero, by the same stipulation,

$$\Phi_2(F) = c \Phi_1(F) \ \forall F \in \mathcal{K}$$

where c is a complex-valued constant, and since Φ_1, Φ_2 both satisfy (2.8), it follows immediately that this is just a constant phase factor $\exp(i\eta)$.

Gauge and Space Translational Covariance. Assume now that the system is subjected to a classical, static magnetic field, of induction

$$B = curl A \tag{2.10}$$

The time-translational automorphisms then become $A-$dependent, and we denote them by $\alpha_A(\mathbf{R})$. We assume that they are covariant w.r.t. space translations and gauge transformations, i.e. that

$$\sigma_0(a) \alpha_A(t) \sigma_0(-a) = \alpha_{A_a}(t); \ \textit{with} \ A_a(x) := A(x-a) \tag{2.11}$$

and

$$(2.12) \qquad \gamma(\frac{e\chi}{\hbar c})\alpha_A(t)\gamma(\frac{-e\chi}{\hbar c}) = \alpha_{A+\nabla\chi}(t)$$

We note now that, in the particular case where B is uniform, it may be represented by the vector potential

$$(2.13) \qquad A = \frac{1}{2}B{\times}x$$

Thus, choosing

$$(2.14) \qquad \chi(x) = -\frac{1}{2}(B{\times}a).x,$$

we see that

$$(2.15) \qquad A + \nabla\chi = A_a$$

Hence, defining $\sigma : X{\rightarrow}Aut(\mathcal{A})$ by the formula

$$(2.16) \qquad \sigma(a) = \gamma(\frac{e\chi}{\hbar c})\sigma_0(a),$$

it follows from (2.11),(2.12) and (2.16) and the definition of $\mathcal{A}$ that σ is a representation of X in $Aut\mathcal{A}$ which commutes with the time translations $\alpha_A(\mathbf{R})$, with the gauge fixed by equn. (2.13). In view of these properties, we take σ to be the space translational automorphisms in the presence of the uniform magnetic field B.

Note. By (2.5),(2.6) and (2.16), the canonical extension of σ to $\mathcal{F}_{el}$, and in particular to the pair field Ψ, yields

$$(2.17) \qquad \sigma(a)\Psi(F) = \Psi(s(a)F)$$

where

$$(2.18) \qquad (s(a)F)(x_1, x_2) = F(x_1 - a, x_2 - a)\exp(\frac{ie(B{\times}a).(x_1 + x_2)}{2\hbar c})$$

Hence,

$$(2.19) \quad [s(a), s(b)]_{\_} = 2isin(\frac{eB.(a{\times}b)}{\hbar c})s(a{+}b) \ and \ s(a)s(-a) = I \ \forall a, b{\in}X$$

where $[,]_{\_}$ denotes commutator. Thus, as $\sigma(a)$ and $\sigma(b)$ do not, in general intercommute, it follows from (2.17) that the extension of $\sigma(X)$ to the field algebra $\mathcal{F}_{el}$ is non- abelian. This is crucial for our derivation of the Meissner effect below.

ODLRO and the Meissner Effect. The essential distinction between normal diamagnetism and the Meissner effect is that the former can support a uniform, static, non-zero magnetic induction and the latter can not. Thus, we base our derivation of the Meissner effect on considerations of the response of an state with ODLRO to the action of a uniform magnetic field.

Proposition 2.2. *The system cannot support uniform, non-zero magnetic induction in translationally invariant states with ODLRO.*

The following Corollary follows immediately from this Propostion and elementary thermodynamics.

Corollary 2.3. *Assuming that translational symmetry is preserved in the equilibrium state* ω_A, *then either*

(1) ω_A *possesses the property of ODLRO and* $B = 0$

or

(2) ω_A *does not possess ODLRO and is normally diamagnetic.*

Further, assuming that, in the absence of a magnetic field, the free energy density of the ODLRO phase is lower, by Δ, *than that of the normal one, the former phase will prevail, and thus the system will exhibit the Meissner effect, provided that the applied field,* H, *satisfies the condition that* $|H| < H_c := (8\pi\Delta)^{1/2}$

Comment. This result signifies that the Meissner effect arises from a rigidity of the macroscopic wave-function in the face of an applied magnetic field. This corresponds precisely to London's [Lo] idea of rigidity, transferred to the macroscopic level.

Proof of Proposition 2.2. By the translational invariance of ω_A and the formula (2.17) for σ,

$$\omega_A(\Psi(s(a)F)^\star\Psi(s(a)G))\equiv\omega_A(\Psi(F)^\star\Psi(G)) \tag{2.20}$$

Further, it follows from the ODLRO condition (2.8) and the definition (2.18) of s that

$$\lim_{y\to\infty}[\omega_A(\Psi(s(a)F)^\star\Psi(s(a)G_y)) - \overline{\Phi(s(a)F)}\Phi(s(a)G_y)] = 0$$

and hence, by (2.20), that

$$\lim_{y\to\infty}[\omega_A(\Psi(F)^\star\Psi(G_y)) - \overline{\Phi_a(F)}\Phi_a(G_y)] = 0 \tag{2.21}$$

where

$$\Phi_a = \Phi \circ s(a) \tag{2.22}$$

Equation (2.21) implies that Φ_a, as well as Φ, serves as a macroscopic wave function for the state ω_A, and therefore, by Lemma 2.1 and equn. (2.22), that

$$\Phi \circ s(a) = c(a)\Phi$$

where $c(a)$ is a complex number of unit modulus. Similarly, if b is another element of X, then

$$\Phi \circ s(b) = c(b)\Phi$$

where $c(b)$ is also a complex number of unit modulus. Thus, the last two equations imply that

$$\Phi \circ [s(a), s(b)]_- = 0$$

On taking the composition product of this equation with $s(-a-b)$ and using (2.19), we see that,

$$sin(\frac{eB.(a \times b)}{\hbar c})\Phi = 0 \ \forall a, b \in X$$

from which it follows that *either* $B = 0$ *or* $\Phi = 0$, which is the required result.

3. Hydrodynamical Phase Transition in a Quantum Plasma.

The quantum Jellium model is a system of electrons, interacting via Coulomb forces both with one another and with a uniform, positively charged, neutralising background. It is thus a model of a many-particle system with realistic interactions. Its thermodynamic properties have been established at the level of mathematical physics [LN]. I shall now sketch a treatment [Se4,7] leading from its many-particle Schrödinger equation to an Eulerian hydrodynamics with a non-equilibrium phase transition. The three principal stages of the derivation of this result are the following. Firstly, we derive a classical Vlasov equation, governing a *large scale* description of its dynamics, from the microscopic Schrödinger equation, together with certain initial and regularity conditions. Secondly, we observe that the Vlasov dynamics corresponds precisely to the Liouville equation for a *Lagrangian* hydrodynamics, governing the evolution of the time (t)-dependent position, $X_t(x)$, of a 'fluid particle'located initially at the point x. Then, finally, we show that this Lagrangian hydrodynamics reduces to a deterministic *Eulerian* form, provided that a certain parameter, governing the non-uniformity in the initial density profile, lies below a certain critical value, and that otherwise it corresponds to a *stochastic* flow.

The Jellium Model, $\Sigma^{(N,L)}$, consists of N electrons in a cube, $K^{(L)}$, of side L, with uniform neutralising positive charge background. We assume periodic boundary conditions. Our objective is to obtain a quantum theoretical derivation of the hydrodynamics of $\Sigma^{(N,L)}$ in a limit where N and L tend to infinity and the mean particle density,

$$\overline{n} = N/L^3 \tag{3.1}$$

remains fixed and finite.

Denoting the gradient operator in $K^{(L)}$ by $\nabla^{(L)}$, we represent the position vectors and momenta of the electrons by the standard multiplicative and differential operators $\{X_j, P_j = -i\hbar\nabla_j^{(L)} | j = 1,..N\}$ in the Hilbert space $\mathcal{H}^{(N,L)}$ of square integrable antisymmetric functions on $(K^{(L)})^N$. The Hamiltonian is then the self-adjoint operator in $\mathcal{H}^{(N,L)}$ given by

$$H^{(N,L)} = \frac{-\hbar^2}{2m}\sum_{j=1}^{N} \Delta_j^{(L)} + e^2 \sum_{j,k(>j)=1}^{N} U^{(L)}(X_j - X_k) \tag{3.2}$$

where $-e, m$ are the electronic charge and mass, respectively, $\Delta^{(L)}$ is the Laplacian for $K^{(L)}$, and $U^{(L)}(X)$ is the difference between $|X|^{-1}$, periodicised w.r.t. $K^{(L)}$, and its space average over that cube, i.e.

$$U^{(L)}(X) = \frac{4\pi}{L^3}\sum^{(L)} \frac{\exp(iQ.X)}{Q^2} \tag{3.3}$$

the superscript (L) over Σ signifying that summation is taken over the nonzero vectors $Q = (2\pi/L)(n_1, n_2, n_3)$, with the n's integers. The pure states of $\Sigma^{(N,L)}$ are represented by the normalised vectors, $\Psi^{(N)}$ in $\mathcal{H}^{(N,L)}$ and their evolution is governed by the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi_T^{(N)}}{\partial T} = H^{(N,L)} \Psi_T^{(N)} \tag{3.4}$$

with T the time variable. We shall assume the following initial kinetic and potential energy bounds for $\Sigma^{(N,L)}$-more precisely, for the family of systems $\{\Sigma^{(N,L)}\}$, with N, L satisfying (3.1).

$(I.1)^{(L)}$ The expectation value of the total kinetic energy per particle, for the initial state $\Psi_0^{(N)}$, is less than some finite $N-$independent constant $B/2m$, i.e.

$$(\Psi_0^{(N)}, P_1^2 \Psi_0^{(N)}) < B \tag{3.5}$$

$(I.2)^{(L)}$ The expectation value of the total potential energy, for the the initial state $\Psi_0^{(N)}$, is less than some finite $N-$independent constant,

$e^2C/2$, times $N^{5/3}$. This bound corresponds to the electrostatic energy of a continuous distribution of charge, whose density is a smooth function of X/L, and signifies that

$$(\Psi_0^{(N)}, U^{(L)}(X_1 - X_2)\Psi_0^{(N)}) < CN^{2/3} \tag{3.6}$$

We base our macroscopic description of the model on scales of length, time and particle momentum given by L, ω^{-1} and $mL\omega$, where ω is the classical plasma frequency, i.e.

$$\omega = (4\pi\overline{n}e^2/m)^{1/2} \tag{3.7}$$

For this description, we employ the rescaled space and time coordinates, $x = X/L$, $t = \omega T$, respectively. Under this rescaling, $\Sigma^{(N,L)}$ is mapped onto a system $\Sigma^{(N)}$ of particles in a unit cube, K, with periodic boundaries. This rescaling induces a unitary mapping of $\mathcal{H}^{(N,L)}$ onto the Hilbert space $\mathcal{H}^{(N)}$ of antisymmetric square integrable functions on K^N, under which $\Psi_T^{(N)}$ is transformed to the state of $\Sigma^{(N)}$ given by

$$\psi_t^{(N)}(x_1, .. ., x_N) = L^{3N/2}\Psi^{(N)}_{\omega^{-1}t}(Lx_1, .. ., Lx_N) \tag{3.8}$$

The Schrödinger equation (3.4) thus transforms to

$$i\hbar_N \frac{\partial \psi_t^{(N)}}{\partial t} = H^{(N)}\psi_t^{(N)} \tag{3.9}$$

where

$$H^{(N)} = \frac{1}{2}\sum_{j=1}^{N} p_j^2 \; + \; N^{-1}\sum_{j,k(>j)=1}^{N} U(x_j - x_k) \tag{3.10}$$

$$p_j = -i\hbar_N \nabla_j \tag{3.11}$$

$$\hbar_N = \frac{\hbar}{mL^2\omega} = \frac{\hbar}{m\omega}(\frac{\overline{n}}{N})^{2/3} \tag{3.12}$$

is a dimensionless effective 'Planck constant', ∇ is the gradient operator for K, and

$$U(x) = \sum_q^{(1)} \exp(iq.x)/q^2 \tag{3.13}$$

the superscript (1) over Σ signifying that summation is taken over the non-zero vectors $2\pi(n_1, n_2, n_3)$, with the n's integers. It follows from (2.13) that

$$\Delta U(x) = 1 - \delta(x) \tag{3.14}$$

where Δ is the Laplacian and δ the Dirac distribution for K.

We formulate the dynamics of $\Sigma^{(N)}$ in terms of its characteristic functions

$$(3.15) \qquad \mu_t^{(N,n)}(\xi_1,..,\xi_n;\eta_1,..,\eta_n) :=$$

$$(\psi_t^{(N)},\Pi_{j=1}^n(\exp(i\xi_j.p_j/2)\exp(i\eta_j.x_j)\exp(i\xi_j.p_j/2))\psi_t^{(N)})$$

where the ξ's and η's run over the ranges $\mathbf{R}^3$ and $(2\pi\mathbf{Z})^3$, respectively.

The initial condition for $\Sigma^{(N)}$, corresponding to $(I.1)^{(L)}$ for $\Sigma^{(N,L)}$, is

$(I.1)$

$$(3.16) \qquad (\psi_0^{(N)},p_1^2\psi_0^{(N)}) < N^{-2/3}b \to 0 \ as \ N\to\infty$$

where b is a finite constant.

The initial condition $(II.2)^{(L)}$ transforms to the following form for $\Sigma^{(N)}$, which is unaffected by the above rephasing of the initial state.

$(I.2)$

$$(3.17) \qquad (\psi_0^{(N)},U(x_1-x_2)\psi_0^{(N)}) < c$$

where c is a finite constant. We further assume that

$(I.3)$

$$(3.18) \qquad \lim_{N\to\infty}\rho_0^{(N,1)}(x) = \sigma_0(x) \ \forall x\in K$$

where the function σ_0 is continuous; and that

$(I.4)$

$$(3.19) \qquad \lim_{N\to\infty}(\mu_0^{(N,n)}(\xi_1,..,\xi_n;\eta_1,..,\eta_n) - \Pi_1^n\mu_0^{(N,1)}(\xi_j,\eta_j))\equiv 0$$

This last condition signifies that, in the limit $N\to\infty$, the initial correlations of $\Sigma^{(N)}$ are of zero range: the assumption behind this is that the initial state of the microscopic model $\Sigma^{(N,L)}$, carries only short range correlations, as in a pure phase [Ru, Se1].

We note here that it was shown by explicit construction, in the Appendix of Ref. [Se7], that the initial conditions (I.1)-(I.4) are perfectly viable.

The macroscopic dynamics of the Jellium model, then, is represented by the time-dependence of the characteristic functions $\mu_t^{(N,n)}$, in the limit $N\to\infty$, subject to the initial conditions (I.1-4).

The Vlasov Dynamics. We note now that the dynamics of the model $\Sigma^{(N)}$, as given by (3.9) and (3.10), has the simplifying features that (a) the effective, dimensionless Planck constant, $\hbar_N$, governing its quantum behaviour, tends to zero as $N \to \infty$; and (b) the pair interaction potential scales as N^{-1}. The properties (a) and (b) are generally the hallmarks of a classical and of a mean field theory, respectively, in the limit $N \to \infty$. In fact, were it not for the Coulomb singularity in U, on e could infer immediately from [NS, Sp] that the Schrödinger equation (3.9), subject to the initial conditions (I.1-4), led to a classical (mean field theoretic) Vlasov dynamics in the limit $N \to \infty$. Specifically, if the two-body potential U in (3.10) were a twice continuously differentiable function, then the following results would prevail.

(A) [NS, Sp] Pointwise convergence of $\mu_t^{(N,1)}$, as $N \to \infty$, to the characteristic function, μ_t, of a classical probability measure m_t on $(K \times \mathbf{R}^3)$, that satisfies the weak Vlasov equation

$$\frac{d}{dt}\int f(x,v)dm_t(x,v) = \int v.\frac{\partial}{\partial x}f(x,v)dm_t(x,v) \tag{3.20}$$

$$-\int \nabla U(x-y).\frac{\partial}{\partial v}f(x,v)dm_t(x,v)dm_t(y,w)\ \forall f \in C_0^2(K \times \mathbf{R}^3)$$

(B) [NS, Sp] Pointwise convergence of $\mu_t^{(N,n)}$ to the characteristic function of the classical probability measure $m_t \otimes m_t .. . \otimes m_t$ $(n\ factors)$ on $(K \times \mathbf{R}^3)^n$.

(C) [Se7] The initial condition for m, ensuing from (I.1) and (I.3), that

$$\int dm_0(x,v)f(x,v) = \int dx\sigma_0(x)f(x,0) \tag{3.21}$$

(D)[Ne, Se7] The unique determination of the solution of the Vlasov equation (3.20), subject to the initial condition (3.21), by that of the Newtonian mean field theoretic problem

$$\frac{dX_t(x)}{dt} = V_t(x);\ \frac{dV_t(x)}{dt} = -\int dy\sigma_0(y)\nabla U'(X_t(x) - X_t(y)); \tag{3.22}$$

$$with\ X_0(x) = x;\ V_0(x) = 0$$

according to the formula

$$\int dm_t(x,v)f(x,v) = \int dx\sigma_0(x)f(X_t(x),V_t(x)) \tag{3.23}$$

In order to extend these results to the Jellium model, $\Sigma^{(N)}$, we require certain regularity conditions on the dynamics of the system, that serve to tame the Coulomb singularity. Accordingly, we invoke certain supplementary assumptions (R), specified in [Se4], whose essential import is that the Coulomb repulsion keeps the electrons apart, sufficiently to ensure that the magnitude of the internal electric field remains bounded. Under these assumptions, we have the following result.

Proposition 3.1.[Se4] *The Schrödinger equation (3.10) for $\Sigma^{(N)}$, together with the initial conditions (I.1-4) and the regularity conditions R, leads to the Vlasov dynamics specified by (A)-(D).*

Eulerian Versus Stochastic Hydrodynamics. The Newtonian mean field theory, given by (3.22), corresponds to a *Lagrangian* hydrodynamics, in which $X_t(x)$ and $V_t(x)$ are the position and velocity, respectively, of a 'fluid particle'; and the Vlasov equation (3.20) is just the Liouville equation representing its probabilistic description. Our aim now is to show that the reducibility of the Vlasov dynamics to a deterministic Eulerian hydrodynamics depends on the invertibility of X_t.

Case (a): X_t Invertible. In this case, the Jacobean

$$J_t(x) = \frac{\partial(X_t^{(1)}, X_t^{(2)}, X_t^{(3)})}{\partial(x^{(1)}, x^{(2)}, x^{(3)})} \tag{3.24}$$

with $x^{(j)}$ (resp. $X_t^{(j)}$) the j'th component x (resp. X_t), is strictly positive, and so we can define

$$\sigma_t(x) = \sigma_0(X_t^{-1}(x))/J_t(x);\ \textit{and}\ u_t(x) = V_t(X_t^{-1}(x)) \tag{3.25}$$

Thus, since, by (3.23) and (3.25),

$$\int dm_t(x,v)f(x,v) = \int dx\sigma_t(x)f(x,u_t(x))\ \forall f\in C(K) \tag{3.26}$$

i.e., formally,

$$dm_t(x,v) = \sigma_t(x)\delta(v - u_t(x))dxdv$$

it follows that $u_t(x)$ and $\sigma_t(x)$ are the drift velocity and normalised particle density, respectively, at position x and time t. Moreover, by (3.14), (3.22) and (3.25), u_t, σ_t evolve according to the Euler-cum-Maxwell hydrodynamical equations

$$\frac{\partial \sigma_t}{\partial t} + \nabla.(\sigma_t u_t) = 0;\ \frac{\partial u_t}{\partial t} + (u_t.\nabla)u_t = E_t;\ \nabla.E_t = (\sigma_t - 1) \tag{3.27}$$

Case (b): X_t Non-Invertible. In this case, we cannot employ the formulae (3.25) to define the time-dependent density and drift velocity. Instead, we have to consider the situation where the equation

$$X_t(y) = x$$

has several solutions, labelled by an index set S, for y as a function of x and t, i.e.

$$y = \{Y_t^{(s)}(x) | s \in S\}$$

In this case, equation (3.26) implies that

$$\int dm_t(x, v) f(x, v) = \sum\nolimits_{s \in S} \int dx \sigma_t^{(s)}(x) f(x, u_t^{(s)}(x)) \tag{3.28}$$

where

$$\sigma_t^{(s)}(x) = \sigma_0(Y_t^{(s)}(x)) |K_t^{(s)}(x)|; \quad u_t^{(s)}(x) = V_t(Y_t^{(s)}(x)) \tag{3.29}$$

and

$$K_t^{(s)}(x) = \frac{\partial(Y_t^{(s,1)}, Y_t^{(s,2)}), Y_t^{(s,3)})}{\partial(x^{(1)}, x^{(2)}, x^{(3)})} \tag{3.30}$$

Thus, (3.28) signifies that the macroscopic state of the system at time t corresponds to a statistical mixture of different streams, indexed by S, with dnsities $\sigma_t^{(s)}$ and drift velocities $u_t^{(s)}$. This implies that the local density and drift velocity of the system are now *stochastic* variables of a hydrodynamics still governed by the Vlasov equation.

We may summarise the above observations in the following form.

Proposition 3.2. *If X_t is invertible, then the macroscopic dynamics of the system corresponds to a deterministic hydrodynamics given by the Euler-cum-Maxwell equations (3.27). Otherwise, it is a stochastic flow, still governed by the Vlasov equation.*

Example of Hydrodynamic Phase Transition. Let us now specialise to the situation where σ_0 is a function of just a single coordinate, $x^{(1)}$. In this case, as the regularity conditions (R) imply uniqueness of the solution of (3.22) [Se4], the flow becomes effectively one-dimensional, with $X_{1,t}$ dependent on the coordinate $x^{(1)}$ only, and $X_t^{(2)}, X_t^{(3)}$ remaining fixed at $x^{(2)}, x^{(3)}$, respectively. For notational convenience, we shall henceforth drop the superscript (1) from $X_t^{(1)}$ and $x^{(1)}$, and denote by $X_t(x)$ the first component of the vector hitherto represented by this symbol. Thus, by equations (3.22),

$$X_t(x) = x + \int_0^t ds(t-s) \int_0^1 dy \sigma_0(y) F(X_s(x) - X_s(y)) \tag{3.31}$$

where

$$(3.32) \qquad F(x) = -\int_0^1 dx^{(2)} \int_0^1 dx^{(3)} \frac{\partial U}{\partial x}(x, x^{(2)}, x^{(3)})$$

Let

$$(3.33) \qquad J_t(x) = \frac{\partial X_t(x)}{\partial x}$$

Then, by Prop. 3.2 and the implicit function theorem, the neccessary and sufficient condition for deterministic hydrodynamics is that J_t has no zeroes. We note also that the definition (3.33) permits us to re-express (3.31) in the form

$$(3.31)' \qquad X_t(x) = x + \int_0^t ds(t-s) \int_0^1 dy \sigma_0(y) F(\int_y^x dz J_s(z)))$$

Proposition 3.3. *Under the specified assumptions, the hydrodynamics of the model is deterministic and given by the Euler-cum-Maxwell equations (3.27), provided that*

$$(3.34) \qquad \sigma_0(x) > \frac{1}{2} \forall x \in [0,1]$$

Otherwise there is a transition to a stochastic flow at a certain time τ, *given by the least positive value of* t *for which*

$$(3.35) \qquad \sigma_0(x) + (1 - \sigma_0(x)) \cos(t) = 0$$

for some $x \in [0,1]$.

Proof. By (3.13), (3.14) and (3.31)-(3.33),

$$(3.36) \quad J_t(x) = 1 + \int_0^t ds(t-s) J_s(x)(-1 + \int_0^1 dy \sigma_0(y) \delta(X_s(x) - X_s(y)))$$

where now δ is the Dirac distribution on $[0,1]$, subject to periodic boundary conditions.

Let us first suppose that X_t is invertible, i.e. that J_t is strictly positive, over a time interval $0 \leq t < \tau_0$, for some positive τ_0. In this case,

$$J_s(x) \delta(X_s(x) - X_s(y)) \equiv \delta(x-y) \ \forall s \in [0, \tau_0)$$

and therefore (3.36) reduces to

$$J_t(x) = 1 + \int_0^t ds(t-s)(\sigma_0(x) - J_s(x))$$

i.e.

$$\left(\frac{d^2}{dt^2}+1\right)J_t(x)=\sigma_0(x);\ with\ J_0(x)=1;\ \dot{J}_0(x)=0$$

where $\dot{J}_t = dJ_t/dt$. Hence,

$$J_t(x)=\sigma_0(x)+(1-\sigma_0(x))\cos(t)$$

In view of the non-negativity of σ_0, this equation implies that J_t is strictly positive for all $t{\geq}0$ if and only if the condition (3.34) is fulfilled. Otherwise, J_t changes sign at some point $x{\in}[0,1]$ when t reaches the value τ specified in the statement of the Proposition. Hence, our assumption of the invertibility of X_t is untenable if (3.34) is violated; and therefore, by Prop. 3.2, the flow becomes stochastic in this case.

The proof (cf. [Se4]) of the converse, i.e. that (3.34) implies the invertibility of X_t and thus the deterministic Euler- cum-Maxwell flow, stems from the explicit form of our regularity condition (R).

4. Macrostatistics and Non-Equilibrium Thermodynamics. Here, I present an approach to the general problem of formulating the structures imposed on non-equilibrium thermodynamics by the underlying quantum mechanics of many-particle systems. This is based on a combination of macroscopic and microscopic treatments of a generic system, Σ, of particles occupying a Euclidean space $X = \mathbf{R}^d$. The argument consists of four parts. The first (§4.1) is a formulation of a mathematical framework for non-equilibrium thermodynamics, based on a macroscopic, continuum mechanical model, M, of Σ. The second (§4.2) is an algebraic quantum statistical formulation of a microscopic model, $\mathcal{Q}$ of the same system. The third (§4.3) consists of a treatment of the connection between M and $\mathcal{Q}$, leading to a *classical macrostatistical mechanics* ($CMSM$) of the observables of $\mathcal{Q}$ that correspond to the hydrodynamical variables of M. This admits a clear formulation of *local equilibrium* conditions and of a generalised version of Onsager's regression hypothesis [On], namely that the macroscopic fluctuations about the flow given by M is governed by the same dynamics as the externally induced 'weak' perturbations to that flow. In §4.4, I derive a generalised form of the Onsager reciprocity relations for M from the structure of $CMSM$. The key elements of this derivation are the symmetry properties of the model, stemming from the microscopic reversibility of $\mathcal{Q}$, and the assumption of local equilibrium.

4.1. The Macroscopic Model, M. In the classical thermodynamical description, the *equilibrium states* of Σ are represented by a certain set $q = (q_1, .. ., q_n)$ of intensive variables, corresponding to global densities of extensive conserved quantities, which we shall characterise in §4.2.

Its entropy density, s, is then a function of these variables, and its equilibrium properties of governed by the form of s. The thermodynamic variables $\theta = (\theta_1, .. ., \theta_n)$ conjugate to q are defined by the formula

$$\theta = \frac{\partial s(q)}{\partial q}, \; i.e. \; \theta_k = \frac{\partial s(q)}{\partial q_k}, \; k = 1, 2.. , n \tag{4.1}$$

and the pressure, p, is the function of θ given by

$$p(\theta) = sup_q(s(q) - q.\theta) \tag{4.2}$$

the dot representing the $\mathbf{R}^n$ inner product. Thus, the inverse of the formula (4.1) (in the pure phase region) is

$$q = -\frac{\partial p(\theta)}{\partial \theta} \tag{4.3}$$

In non-equilibrium thermodynamics, the state of the system is generally not translationally invariant, and the macroscopic variables q become functions of position, x, and of time, t. In other words, the macrostate is an n-component *classical field*

$$q(x, t) \equiv q_t(x) \equiv (q_{1,t}(x), .. ., q_{n,t}(x)).$$

The laws of continuum mechanics, such as those of hydrodynamics or heat conduction, are then of the *deterministic* form

$$\dot{q}_t = \mathcal{F}(q_t) \tag{4.4}$$

where $\mathcal{F}$ is some functional of the fields q_t. Equivalently, defining the local thermodynamic conjugates θ_t of the fields q_t by

$$\theta_t(x) \equiv \theta(x, t) := \frac{\partial s(q(x, t))}{\partial q}, \tag{4.5}$$

it follows from (4.3) that the equation of motion (4.4) may be re-expressed as

$$\dot{q}_t \equiv \frac{d\dot{q}_t}{dt} = \Phi(\theta_t); \; \Phi := \mathcal{F} \circ (-\frac{\partial p}{\partial \theta}) \tag{4.6}$$

Note. The definition (4.5) of θ_t does not require the microstate of Σ to simulate one of equilibrium at a local level. On the other hand, some assumption of local equilibrium will be needed for the determination of properties of the functional $\mathcal{F}$.

Example. An example of a law of the above form is the non- linear, n-component diffusion given by

$$\dot{q}_{k,t} = \sum_{l=1}^{n} \nabla.(L_{k,l}(\theta_t)\nabla\theta_{l,t}) \tag{4.6a}$$

Returning to the general structure, we impose the following assumptions on the dynamical law (4.6).

(M.1) *The system is confined to a single phase region, i.e. the values of* $q_t(x)$, $\theta_t(x)$ *always lie in domains where the functions* s *and* p *are* $C^{(\infty)}$.

(M.2) $\mathcal{F}(q) = 0$ *if* $q(x)$ *is constant, i.e. the system is in equilibrium if its local thermodynamic variables* $q(x)$ *(or equivalently* $\theta(x)$*) are spatially uniform.*

(M.3) *The equation of motion (4.6) is covariant w.r.t. space-time translations and scale transformations* $x\to\lambda x, t\to\lambda^r t$, *with* r *a positive integer (=2 in the case of (4.6a)).**

Let y_t, η_t be 'small' perturbations of q_t, θ_t, respectively, and let

$$[\Lambda(\theta)\eta_t](x) := \frac{d}{dz}\Phi(\theta_t(x) + z\eta_t(x))|_{z=0} \tag{4.7}$$

in the pointwise sense, for the class of functions η_t for which the r.h.s. of this formula is well-defined. Then it follows from (4.6) and (4.7) that the *linearised* equation of motion for y_t is

$$\dot{y}_t = \mathcal{L}(\theta_t)y_t \tag{4.8}$$

where

$$\mathcal{L}(\theta_t) = \Lambda(\theta_t)B(\theta_t) \tag{4.9}$$

and $B(\theta)$ is the Hessian $s''(q)$, i.e.

$$(B(\theta))y)_k := \sum_{l=1}^{n} \frac{\partial^2 s(q)}{\partial q_k \partial q_l} y_l \tag{4.10}$$

The next assumption permits us to formulate the perturbed dynamics as the evolution of a tempered distribution. Thus, defining $\mathcal{S}^{(n)}(X)$ to be the

* Note that this assumption is not always fulfilled: for example, the Navier-Stokes equation is not scale invariant.

space of the Schwartz $\mathcal{S}-$class $\mathbf{R}^n-$ valued functions on X, and $\mathcal{S}^{(n)\prime}(X)$ to be its dual space, we assume that

(M.4) *the linear operator* $\mathcal{L}(\theta_t)$ *extends, by continuity, to a transformation of* $\mathcal{S}^{(n)\prime}(X)$, *and the formula (4.8), considered now as an equation of motion in that space, has a unique solution*

$$y_t = T(\theta_.|t,t')y_{t'} \ \forall t \geq t' \geq 0 \tag{4.11}$$

with

$$T(\theta_.|t,t_0) \equiv T(\theta_.|t,t_1)T(\theta_.|t_1,t_0) \ and \ T(\theta_.|t,t) = 1 \ \forall t \geq t_1 \geq t_0 \geq 0$$

Comments. In the equilibrium case, where $\theta_t = \overline{\theta}$, a constant, the two-parameter family $T(\theta|.,.)$ of transformations of $\mathcal{S}^{(n)\prime(X)}$ reduces to a one-parameter semi-group $\{\tilde{T}(\overline{\theta}|t)|t \in \mathbf{R}_+\}$, where

$$\tilde{T}(\overline{\theta}|(t-t_0) \equiv T(\overline{\theta}|(t,t_0) = \exp(\mathcal{L}(\overline{\theta})(t-t_0)) \tag{4.12}$$

Further, in the case of the non-linear diffusion (4.6a), $\mathcal{L}(\theta^{(0)})$ reduces to the form

$$\mathcal{L}(\overline{\theta}) = L(\overline{\theta})B(\overline{\theta})\Delta; \ L(\overline{\theta}) = [L_{kl}(\overline{\theta})]; \ B = [B_{kl}(\overline{\theta})] \tag{4.12a}$$

where Δ is the Laplacian.

The following Proposition follows immediately from (M.1) and (M.4).

Proposition 4.1. *The process* $y.$ *is covariant w.r.t. space translations and space-time scale transformations, i.e. defining*

$$\phi_t^{(a,b,\lambda)}(x) \equiv \phi^{(a,b,\lambda)}(x,t) := \phi(a+\lambda x, b+\lambda^r t), \ for \ \phi = \theta, q, y \tag{4.13}$$

and for arbitrary $(a,b,\lambda) \in X \times \mathbf{R} \times \mathbf{R}_+$),

$$(T(\theta_.|t,t')y_{t'})^{(a,b,\lambda)} \equiv T(\theta_.^{(a,b,\lambda)}|t,t')y_{t'}^{(a,b,\lambda)} \tag{4.14}$$

4.2. The Quantum Model, $\mathcal{Q}$. In order to accommodate the dynamics of both the microscopic and macroscopic observables of Σ, we construct its quantum model, $\mathcal{Q}$, as a $W^\star-$dynamical system [Se6] $(\mathcal{A}, \alpha, \mathcal{N}(\mathcal{A}))$, where $\mathcal{A}$ is a $W^\star-$algebra of observables, $t \rightarrow \alpha_t$ is a representation of $\mathbf{R}$ in $Aut(\mathcal{A})$, corresponding to the dynamics of the system, and $\mathcal{N}(\mathcal{A})$) is the folium of normal states on $\mathcal{A}$. In fact, this algebra is constructed as the weak closure of the largest locally normal representation, π, of the standard [HHW] quasi-local $C^\star-$algebra, $\tilde{\mathcal{A}}$, that can support the dynamical and thermodynamical structures we require. Thus, we characterise $\mathcal{A}, \alpha$ and π according to the following prescription.

(1) Let L be the set of bounded open regions of X. Then for each $\Lambda \in L$, there is a type-I factor, $\mathcal{A}(\Lambda)(\subset \mathcal{A})$, representing the observables of that region and satisfying the conditions of isotony and local commutativity; and $\mathcal{A}$ is the weak closure of $\mathcal{A}_L := U_{\Lambda \in L} \mathcal{A}(\Lambda)$. We extend automorphisms γ of $\mathcal{A}$ to unbounded observables, Q, affiliated* to this algebra, according to the formula

$$\exp(i\lambda\gamma(Q)) = \gamma(\exp(i\lambda Q)) \ \forall \lambda \in \mathbf{R} \tag{4.15}$$

We similarly extend anti-automorphisms of $\mathcal{A}$ to its unbounded affiliates.

(2) The local energy observable (Hamiltonian) $H(\Lambda)$ for the region $\Lambda(\in L)$ is, in general, an unbounded one, affiliated to $\mathcal{A}(\Lambda)$. We assume that $\mathcal{A}$ is equipped with a Wigner time-reversal anti-automorphism, ρ, which leaves this observable invariant, i.e.

$$\rho H(\Lambda) = H(\Lambda) \tag{4.16}$$

(3) Space translations are represented by a homomorphism σ of X into $Aut(\mathcal{A})$, such that $\sigma(x)\mathcal{A}_0(\Lambda) \equiv \mathcal{A}_0(\Lambda + x)$ and $\sigma(x)H(\Lambda) = H(\Lambda + x))$, this last condition representing an assumption of translationally invariant interactions.

(4) The dynamical automorphisms α are given by infinite volume limits of those of finite versions of Σ, according to the formula

$$\alpha_t A = s - \lim_{\Lambda\uparrow}(\exp(iH(\Lambda)t/\hbar)A\exp(-iH(\Lambda)t/\hbar)) \ \forall t \in \mathbf{R}, \ A \in \mathcal{A}_L \tag{4.17}$$

Thus, by the translational covariance of $H(\Lambda)$, α_t commutes with the space translational automorphisms, σ, and, by (4.16), satisfies the *microscopic reversibiliy* condition

$$\rho\alpha_t\rho = \alpha_{-t} \ \forall t \in \mathbf{R} \tag{4.18}$$

(5) We formulate the thermodynamics of the system in terms a Hermitian quantum field $\hat{q} = (\hat{q}_1, .. ., \hat{q}_n)$, the $\hat{q}_k' s$ being densities of locally conserved quantities. We assume that $\hat{q}$ is a tempered distribution, affiliated to $\mathcal{A}$, that transforms covariantly w.r.t space translations. Thus, $\hat{q}$ is a mapping of $\mathcal{S}^{(n)}(X)$ into the self-adjoint affiliates of $\mathcal{A}$. We assume

* Recall that, if $\mathcal{M}$ is a $W^\star-$algebra of operators in a Hilbert space $\mathcal{H}$, then the unbounded operators, in $\mathcal{H}$, affiliated to $\mathcal{M}$ are the densely defined ones that commute with $\mathcal{M}'$.

that the function $\exp(i\hat{q}(.))$ is strongly continuous, and that $\hat{q}$ transforms covariantly w.r.t. space translations, i.e.

$$\sigma(x)[\hat{q}(f)] = \hat{q}(f_x), \ \textit{where} \ f_x(y) = f(x-y) \ \forall x, y \in X, f \in \mathcal{S}^{(n)}(X) \tag{4.19}$$

We assume, for simplicity, that $\hat{q}$ is invariant under time reversals, i.e.

$$\rho\hat{q}(f) \equiv \hat{q}(f) \tag{4.20}$$

and that its components satisfy the following commutation relations, which signify that their space integrals over finite volumes intercommute, up to 'surface effects'.

$$[\hat{q}_k(g), q_l(h)]_- = i\hbar j_{k,l}(\nabla(gh)) \ \forall g, h \in \mathcal{S}(X), \tag{4.21}$$

where $(gh)(x) := g(x)h(x)$ and $j_{k,l}$ a tempered distribution. Further, denoting $\alpha_t[\hat{q}(f)]$ by $\hat{q}_t(f)$, we assume local conservation law of the form

$$\frac{\partial \hat{q}_t(f)}{\partial t} = j_t(\nabla f) \tag{4.22}$$

where j_t is a tempered distribution.

(6) We take the equilibrium thermodynamic variables of $\mathcal{Q}$ to be the 'observables at infinity' [LR], given by the global spatial average $\hat{q}^{\infty}$ of $\hat{q}$ over X. Further, denoting by $\hat{s}$ the standard [Ru] entropy density functional on the translationally invariant states on $\mathcal{A}_0$, we assume that these observables form a complete thermodynamic set, in the sense that [Se1, Ch.4]

(a) for each expectation value, q, of $\tilde{q}$, there is precisely one translationally invariant state ($\in\mathcal{N}(\mathcal{A})$) that maximises $\hat{s}$; and

(b) no proper subset of $\hat{q}$ possesses this property.

The equilibrium thermodynamics of the system is thus given by the form of the resultant entropy density, $s(q)$. We identify q, s with the objects denoted by these symbols in the macroscopic model M; and, defining θ according to (4.1), we denote by ω_θ the maximising state of condition (a). We assume that this state is stationary,* i.e. $\alpha-$invariant, in view of the fact that $\hat{q}_\infty$ is a globally conserved quantity; and we designate it as the equilibrium state corresponding to θ, i.e. to q. We note that, by (4.18) and the thermodynamic completeness condition (a),

$$\omega_\theta \circ \rho = \omega_\theta \tag{4.23}$$

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* The proof of this is straightforward for lattice systems, since one can show within the framework of [Se1,Ch.4], that, for these, ω_θ satisfies the KMS conditions, and is therefore stationary.

(7) We define π to be the largest locally normal representation of $\tilde{\mathcal{A}}$ that supports the dynamical group α and the quantum field $\hat{q}$, as defined above.

Thus, the quantum model, $\mathcal{Q}$, is given by $(\mathcal{A}, \alpha, \sigma, \hat{q}, \mathcal{N}(\mathcal{A}))$, as specified by the conditions (1)-(7).

4.3. Relationship between M and $\mathcal{Q}$. Our formulation of this relationship is based on the idea that the phenomenological law (4.6) corresponds to the dynamics of the quantum field $\hat{q}$ in a large-scale limit. Thus, in view of the scale-invariance assumption (M.1) for M, we introduce a length parameter L and reformulate $\mathcal{Q}$ on a length scale L and a time scale L^r, defining the quantum field $\hat{q}^{(L)}$ on these scales by the formula

$$(4.24) \qquad \hat{q}_t^{(L)}(f) \equiv \hat{q}^{(L)}(f,t) := \hat{q}(f^{(L)}, L^r t)$$

where

$$(4.25) \qquad f^{(L)}(x) := L^{-d} f(x/L)$$

We assume that L is also the length scale of spatial variations of the initial state, $\omega^{(L)}$, of $\mathcal{Q}$, i.e. that there is a map $A \rightarrow \overline{A}$ of $\mathcal{A}$ into $C(X)$ and a tempered distribution $q_0 (\in \mathcal{S}^{(n)\prime})$, such that

$$(4.26) \qquad \lim_{L\to\infty} \omega^{(L)}(\sigma(Lx)[A]) = \overline{A}(x) \ \forall x \in X$$

and

$$(4.27) \qquad \lim_{L\to\infty} \omega^{(L)}(\hat{q}_0^{(L)}(f)) = q_0(f) \ \forall f \in \mathcal{S}^{(n)}$$

We define the fluctuation field $\hat{\xi}^{(L)}$ by the formula

$$(4.28) \qquad \hat{\xi}_t^{(L)}(f) := L^{d/2}(\hat{q}_t^{(L)}(f) - \omega^{(L)}(\hat{q}_t^{(L)}(f))), \ \forall f \in \mathcal{S}^{(n)}(X), \ t \in \mathbf{R}$$

Our basic assumptions for the large-scale dynamics of the model are the following.

(I) *For each $M-$ process $q_{.}$, there is an equivalence class of initial states, $\{\omega^{(L)}\}$, parametrised by L, such that*

(a) the mapping

$$f^{(1)}, .. ., f^{(m)}; t^{(1)}, . ., t^{(m)} \rightarrow \omega^{(L)}(\hat{\xi}_{t^{(1)}}^{(L)}(f^{(1)}) .. .(\hat{\xi}_{t^{(m)}}^{(L)}(f^{(m)}))$$

of $(\mathcal{S}^{(n)})^m \times \mathbf{R}^m)$ into $\mathbf{C}$ is continuous, for all positive integers m.

(b) The expectation value of the quantum field $\hat{q}_t^{(L)}$ reduces to that of the classical one, q_t, of M in the limit $L\to\infty$, i.e.

$$(4.29)\qquad \lim_{L\to\infty}\omega^{(L)}(\hat{q}_t^{(L)}(f))) = q_t(f)\ \forall f\in\mathcal{S}^{(n)}(X)$$

where q_t is the solution of (4.4), with initial value given by (4.27).

(c) The quantum stochastic process $\hat{\xi}^{(L)}$ converges to a classical one, ξ, as $L\to\infty$, i.e.

$$(4.30)\qquad \lim_{L\to\infty}\omega^{(L)}(\hat{\xi}_{t^{(1)}}^{(L)}(f^{(1)}).. .(\hat{\xi}_{t^{(m)}}^{(L)}(f^{(m)})) =$$

$$\mathbf{E}[\theta_{.}|(\xi_{t^{(1)}}(f^{(1)}).. .\xi_{t^{(m)}}(f^{(m)})]$$

$$\forall t^{(1)},. .,t^{(m)}\in\mathbf{R}_+,\ f^{(1)},.. .,f^{(m)}\in\mathcal{S}^{(n)}(X),\ r\in\mathbf{N}$$

where the expectation functional $\mathbf{E}[\theta_{.}|.]$ is governed by the restriction of $\theta_{.}$ to the close interval between the minimum and maximum of $\{t^{(1)},. .,t^{(m)}\}$.

Comments. (1) The classicality of the limits of $q^{(L)}$ and $\xi^{(L)}$ here are assumed to arise from the commutation rules (4.21), together with asymptotic abelian properties of $\mathcal{Q}$ with respect to time.

(2) Since (c) implies that the dispersion in $\hat{q}_t^{(L)}$, for the state $\omega^{(L)}$, tends to zero as $L\to\infty$, it follows from (b) that the quantum process $\hat{q}_t^{(L)}$ reduces to the classical one, q_t, in this limit.

(3) It follows from (b) and (c) that ξ_t is an $\mathcal{S}^{(n)\prime}-$valued random variable.

Let

$$(4.31)\qquad \omega_{\tau}^{(L)} := \omega^{(L)}\circ\alpha(L^r\tau)\ \forall\tau\in\mathbf{R}_+$$

Then $\{\omega_t^{(L)}\}$ satisfies the conditions of (I), and the replacement of $\omega^{(L)}$ by $\omega_{\tau}^{(L)}$ corresponds to that of $\theta_{.}$ by $\theta^{(\tau)}$ in (4.30), where

$$(4.32)\qquad \theta_t^{(\tau)} = \theta_{t+\tau},\ \forall t,\tau\in\mathbf{R}_+$$

i.e.

$$(4.33)\qquad \mathbf{E}[\theta_{.}|(\xi_{t^{(1)}+\tau}(f^{(1)}).. .\xi_{t^{(m)}+\tau}(f^{(m)})]\equiv$$

$$\mathbf{E}[\theta_{.}^{(\tau)}|(\xi_{t^{(1)}}(f^{(1)}).. .\xi_{t^{(m)}}(f^{(m)})]$$

In the particular case where $t^{(1)} = .. = t^{(m)} = 0$, the r.h.s. of this equation depends on $\theta_{.}^{(\tau)}$ only through the value of $\theta_0^{(\tau)}\equiv\theta_{\tau}$, by (4.32). Thus, by

(4.30), the equal time correlation functions for the process $\xi_.$ are of the form

$$\mathbf{E}[\theta_.|\xi_\tau(f^{(1)}).. .\xi_\tau(f^{(m)})]\equiv\mathbf{E}[\theta_\tau|\xi_0(f^{(1)}).. .\xi_0(f^{(m)})] \tag{4.34}$$

Our next assumption is that the space-time clustering properties of $\mathcal{Q}$ render the process $\xi_.$ Gaussian (cf. [GVV]), and that the infinite separation of the relevant relaxation time-scales of the models M and $\mathcal{Q}$ ensure that it is Markovian.

(II) *The process $\xi_.$ is Gaussian and temporally Markovian.*

It follows immediately from this assumption that the process ξ is completely determined by its two-point function. Our next assumption is the following generalisation of Onsager's regression hypothesis [On].

(III) *The fluctuation process ξ is governed by precisely the same dynamics as the perturbation, $y_.$, to the deterministic process $q_.$, i.e., by (4.11),*

$$\mathbf{E}[\theta_.|(\xi_{t+\tau}(f)\xi_t(g)] = \mathbf{E}[\theta_.|(\xi_t(T(\theta_.|t+\tau,t)^\star f)\xi_t(g)]$$

Hence, by (4.34)

$$\mathbf{E}[\theta_.|(\xi_{t+\tau}(f)\xi_t(g)] = \mathbf{E}[\theta_t|(\xi_0(T(\theta_t|t+\tau,t)^\star f)\xi_0(g)] \tag{4.35}$$

$$\forall f\in\mathcal{S}^{(n)}(X), t\in\mathbf{R},\ \tau\in\mathbf{R}_+$$

Thus, the process is determined by the form of T and of the expectation functional $\mathbf{E}[\theta_t|.]$ on the algebra generated by ξ_0. In order to formulate the action of space translations and scale transformations on the process, we define

$$f^{(a,\lambda)}(x) := \lambda^{-d/2}f(\lambda^{-1}(x-a))\ \forall a\in X, \lambda\in\mathbf{R}_+ \tag{4.36}$$

and

$$\xi_0^{(a,\lambda)}(f) := \xi_0(f^{(a,\lambda)})\ \forall a\in X, \lambda\in\mathbf{R}_+ \tag{4.37}$$

Proposition 4.2 *Under the above assumptions and definitions,*

$$\mathbf{E}[\theta_b|(\xi_0^{(a,\lambda)}(T(\theta_.|b+\tau,b)^\star f)\xi_0^{(a,\lambda)}(g)] = \tag{4.38}$$

$$\mathbf{E}[\theta_0^{(a,b,\lambda)}|\xi_0(T(\theta_.^{(a,b,\lambda)}|\tau,0)^\star f)\xi_0(g)]\ \forall a\in X,\ b,\tau\in\mathbf{R}_+,\ \lambda\in\mathbf{R}_+$$

with $\theta_.^{(a,b,\lambda)}$ as defined by (4.13).

Proof. The result is obtained by replacing each f by $f^{a\lambda}$, in (4.30), and using equns. (4.13), (4.14), (4.19), (4.27), (4.28), and (4.35)-(4.37).

We note now that the local properties of the process ξ, in the neighbourhood of a space-time point (a,b), is given by the form of the l.h.s. of (4.38), in the limit $\lambda\rightarrow 0$. Moreover, by (4.13), the function $\theta_{.}^{(a,b,\lambda)}$, which occurs there, tends pointwise to a constant, $\theta(a,b)$, in this limit. These observations leads us to the following *local equilibrium* assumption.

(V)

$$\text{(4.39)} \qquad \lim_{\lambda\rightarrow 0}\mathbf{E}[\theta_0^{(a,b,\lambda)}|\xi_0(T(\theta_{.}^{(a,b,\lambda)}|(\tau,0)^\star f)\xi_0(g)] =$$

$$\mathbf{E}[\theta(a,b)|(\xi_0(T(\theta(a,b)|\tau,0)^\star f)\xi_0(g)] \ \forall f,g\in\mathcal{S}^{(n)}(X), \ \tau\geq 0$$

and further, the r.h.s. of this formula is precisely the same as for the fluctuations of the field $\hat{q}_{.}$ about an equilibrium state $\omega_{\theta(a,b)}$, as defined in item (6) of §4.2, *i.e.*

$$\text{(4.40)} \qquad \mathbf{E}[\theta(a,b)|\xi_0(T(\theta(a,b)|\tau,0)^\star f)\xi_0(g)]\equiv$$

$$\lim_{L\rightarrow\infty}\omega_{\theta(a,b)}([\alpha(L^r\tau)\hat{\xi}_0(f)]\hat{\xi}_0(g))$$

Hence, by (4.12) and (4.40),

$$\text{(4.41)} \qquad \mathbf{E}[\theta(a,b)|\xi_0(\exp(\mathcal{L}(\theta(a,b))\tau))^\star f)\xi_0(g)] =$$

$$\lim_{L\rightarrow\infty}\omega_{\theta(a,b)}([\alpha(L^r\tau)\hat{\xi}_0(f)]\hat{\xi}_0(g))$$

4.4. Consequences of (I)-(V): Generalised Onsager Relations. Let $\mathcal{R}(\theta)$ be the range of the function $\theta\equiv\{\theta(a,b)|a\in X, b\in\mathbf{R}_+\}$. We shall employ the above theory to obtain properties of $\mathbf{E}[\overline{\theta}|.]$ and $\mathcal{L}(\overline{\theta})$ for arbitrary $\overline{\theta}\in\mathcal{R}(\theta)$.

(a) **Symmetry Property of Time Correlations Functions.** In view of the microscopic reversibility conditions (4.18), (4.20) and (4.23), together with the stationarity of $\omega_{\overline{\theta}}$, it follows from (4.30), with $\omega^{(L)}=\omega_{\overline{\theta}}$, that

$$\omega_{\overline{\theta}}(\xi_t(f)\xi_0(g))\equiv\omega_{\overline{\theta}}(\xi_0(f)\xi_{-t}(g))\equiv\omega_{\overline{\theta}}(\xi_t(g)\xi_0(f)) \ \forall\overline{\theta}\in\mathcal{R}(\theta)$$

Hence, by (4.41), we have the symmetry property

$$\text{(4.42)} \quad \mathbf{E}[\overline{\theta}|\xi_0(\exp(\mathcal{L}(\overline{\theta})^\star\tau)f)\xi_0(g)]\equiv\mathbf{E}[\overline{\theta}|\xi_0(\exp(\mathcal{L}(\overline{\theta})^\star\tau)g)\xi_0(f)] \ \forall\overline{\theta}\in\mathcal{R}(\theta)$$

(b) **The Static Two-point Function.** It follows immediately from (4.41) that $\mathbf{E}[\overline{\theta}|.]$ inherits the translational invariance of $\omega_{\overline{\theta}}$. Hence, in view of the tempered distribution property of ξ_0, the generalised function $(x,y)(\in X^2)\rightarrow\mathbf{E}[\overline{\theta}|(\xi_0(x)\xi_0(y)]$ is an $\mathcal{S}^{(n)\prime}(X)-$ class distribution $F(x-y)$; and, by Prop. 4.2, $F(\lambda x)\equiv\lambda^{-d}F(x)$, and is therefore of the form $C\delta(x)$, where C is an n-by-n matrix. Thus,

$$\mathbf{E}[\overline{\theta}|\xi_0(f)\xi_0(g)] = \langle Cf, g\rangle \ \forall\overline{\theta}\in\mathcal{R}(\theta) \tag{4.43}$$

where the angular brackets denote the inner product for the Hilbert space $\mathcal{H}^{(n)}$ of square integrable functions from X into $\mathbf{R}^n$, as defined by the formula

$$\langle f, g\rangle = \int f(x).g(x)dx \tag{4.44}$$

the dot denoting the $\mathbf{R}^n$ scalar product. Moreover, it follows [Se5] from a treatment of the linear response of $\omega_{\overline{\theta}}$ to local Hamiltonian perturbations $\hat{q}(f)$ that, under mild technical assumptions, $C = B(\theta)^{-1}$, where B is specified in (4.10). Hence, by (4.43),

$$\mathbf{E}[\overline{\theta}|\xi_0(f)\xi_0(g)] = \langle B(\overline{\theta})^{-1}f, g\rangle \tag{4.45}$$

(c) **Generalised Onsager Relations.** It follows immediately from (4.42) and (4.45) that

$$\langle B(\overline{\theta})^{-1}\exp(\mathcal{L}(\overline{\theta})^{\star}\tau)f, g\rangle\equiv\langle B(\overline{\theta})^{-1}\exp(\mathcal{L}(\overline{\theta})^{\star}\tau)g, f\rangle \tag{4.46}$$

Hence, by (4.9), we have the following result.

Proposition 4.3. *Under the above assumptions,* Λ *satisfies the generalised Onsager relation*

$$\langle\Lambda(\overline{\theta})^{\star}f, g\rangle\equiv\langle\Lambda(\overline{\theta})^{\star}g, f\rangle \ \forall\overline{\theta}\in\mathcal{R}(\theta), \ f, g\in\mathcal{S}^{(n)\prime}(X) \tag{4.47}$$

i.e. $\Lambda(\overline{\theta})$, *considered as an operator in* $\mathcal{H}^{(n)}$, *with domain* $\mathcal{S}^{(n)}$, *is symmetric.*

Comment. In the case of the non-linear diffusion given by (4.6a), it follows from (4.12a) that (4.47) reduces to the form

$$L_{kl}(\theta)(x,t)) = L_{lk}(\theta)(x,t)) \ \forall x\in X, \ t\in\mathbf{R}_+$$

5. Concluding Remarks. I have endeavoured to show here how, at least in certain domains, a macroscopically-based approach to statistical mechanics can serve to determine the form imposed by quantum mechanics on the structure of phenomenological laws. By contrast with the standard many-body theory, the microscopic imput here is limited to very general principles; and this serves to pare down the conceptual structure of the theory to its essentials.

Of course, the relative simplicity gained by this approach is dependent on a number of assumptions, specified in the previous Sections, that are very difficult to verify constructively. Furthermore, the dynamical systems treated in $\S's$ 3 and 4 have the simplifying, and rather particular, property of scale covariance. In the case of the plasma model, this stems from the fact that the Coulomb potential is given by a power law: in the case of the non-equilibrium thermodynamics of §4, it is an assumed property of the macroscopic dynamics.

Thus, it is clear that the formulation of a coherent, general formulation of the statistical mechanics of macroscopic variables poses deep problems, concerning both its underlying assumptions and its potential scope. I would hope that inroads into these problems may be achieved through the study both of suitable models and of the relevant general structures.

References

[An] P. W. Anderson: Phys. Rev. **110**, 827 (1959)

[BCS] J. Bardeen, L. N. Cooper and J. R. Schrieffer: Phys. Rev. **108**, 1175 (1957)

[DF] B. Deaver and W. M. Fairbank: Phys. Rev. Lett. **7**, 43 (1961)

[GVV] D. Goderis, A. Verbeure and P. Vets: Pp. 178-193 of "Quantum Theory and Applications V", Ed. L. Accardi and W. von Waldenfels, Springer Lecture Notes in Mathematics 1442, 1990

[He] K. Hepp: Helv. Phys. Acta **45**, 237 (1972)

[HL] K. Hepp and E. H. Lieb: Helv. Phys. Acta **46**, 973 (1073)

[HHW] R. Haag, N. M. Hugenholtz and M. Winnink: Commun. Math. Phys. **5**, 215 (1967)

[Jo] B. D. Josephson: Rev. Mod. Phys. **36**, 216 (1964)

[Lo] F. London: Superfluids, Vol. 1, Wiley, London, 1950

[LL] L. D. Landau and I. M. Lifschitz: "Fluid Mechanics", Pergamon Press, Oxford, New York, Paris, 1984

[LN] E. H. Lieb and H. Narnhofer: J. Stat. Phys. **12**, 291 (1975)

[LR] O. E. Lanford and D. Ruelle: Commun. Math. Phys. **13**, 194 (1969)

[Ne] Fluid Dyn. Trans. **9**,229 (1978)

[NS] H. Narnhofer and G. L. Sewell: Commun. Math. Phys. **79**, 9 (1981)

[On] L. Onsager: Phys. Rev. **37**, 405 (1931) and **38**, 2265 (1931)

[Pe] O. Penrose: Phil. Mag. **42**, 1373 (1951)

[PO] O. Penrose and L. Onsager: Phys. Rev. **104**, 576 (1956)

[Ri] G. Rickayzen: Phys. Rev. **115**, 795 (1959)

[Ru] D. Ruelle: "Statistical Mechanics", W. A. Benjamin Inc., New York, 1969 [Sc] M. R. Schafroth: Phys. Rev. **100**, 463 (1955)

[Se1] G. L. Sewell: "Quantum Theory of Collective Phenomena", Oxford University Press, Oxford, 1989

[Se2] G. L. Sewell: J. Stat. Phys. **61**, 415 (1990)

[Se3] G. L. Sewell: "Macroscopic Quantum Theory of Superconductivity and the Higgs Mechanism", to be published in the Proceedings of the 1991 Locarno Conference on "Stochastics, Physics and Geometry".

[Se4] G. L. Sewell: "Quantum Plasma Model with Hydrodynamical Phase Transition", Preprint

[Se5] G. L. Sewell:Pp.77-122 of "Large-Scale Molecular Systems: Quantum and Stochastic Aspects", Nato ASI Series B, Ed. W. Gans, A. Blumen and A. Amann, Plenum, New York and London, 1991

[Se6] G. L. Sewell: Lett. Math. Phys. **6**, 209 (1982)

[Se7] G. L. Sewell: J. Math. Phys. **26**, 2324 (1985)

[Sp] H. Spohn: Math. Meth. Appl. Sci. **3**,445 (1981)

[Ya] C. N. Yang: Rev. Mod. Phys. **34**, 694 1962

[ZA] Z. Zou and P. W. Anderson: Phys. Rev. B **37**, 627 (1987)

TOWARDS A MACROSTATISTICAL MECANICS*

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ABSTRACT

I discuss the general question of the derivation of the statistical mechanics of macroscopic variables from the quantum structures of many-particle systems, as represented in the thermodynamic limit. I then present a number of strands of such a macrostatistical mechanics, including (a) a derivation of the electrodynamics of superconductors from their order structure and gauge covariance; (b) a hydrodynamics, with transition from deterministic to stochastic flow, of a quantum plasma model; and (c) a non-linear generalisation of Onsager's irreversible thermodynamics.

1. Introduction. The 'miracle' of statistical physics is that the microscopically chaotic dynamics of many-particle systems conspires to generate macroscopic laws of relatively simple structure, such as those of thermodynamics and hydrodynamics. In view of the complexity of the microscopic picture and the simplicity of the macroscopic one, it is natural to seek an approach to the subject, that is centred on macro- observables, with microscopic imput limited to very general principles, e.g. conservation laws, ergodicity, etc. Such an approach would evidently be at the opposite pole from the conventional microscopically based 'many-body theory'.

In fact, there are already important macroscopically-based theories in statistical physics, most notably Onsager's [On] linear irreversible thermodynamics and Landau's [LL, Ch.17]] fluctuating hydrodynamics. However, these theories are essentially heuristic because, apart from questions of rigour, they lack the structures needed for a precise characterisation of their purportedly key ingredient of macroscopicality. Moreover, the same thing can be said about all works devised within the traditional framework of the statistical mechanics of strictly finite systems.

On the other hand, the 'revolution' in statistical mechanics, based on the formulation of many-particle systems in the thermodynamic limit [Ru, HHW, He], have provided us with just the framework required for a sharp characterisation of macroscopicality, and even of different levels thereof [Se1, GVV]. My objective here is to discuss the project of extracting a 'macrostatistical mechanics' (MSM) from the quantum structures of many-particle systems, within this framework. In fact, we already have some strands of such a discipline in the works of Hepp and Lieb [HL] on the derivation of the macroscopic dynamics, with non-equibrium phase transition, of a laser mode; of myself [Se1,Ch.4] on the formulation of an extended classical thermodynamics with phase structure; and of the Leuven school [GVV] on macroscopic fluctuation theory.

In this article, I shall bring together further contributions, from three different areas, towards an MSM. The first of these, (§2), consists of a derivation of the electromagnetic properties of superconductors from their order structure and gauge covariance [Se2,3]. The second, (§3), is an extraction of the hydrodynamics, with non-equilibrium phase transition, of a quantum plasma model [Se4]; and the third, (§4), consists of a quantum-statistical derivation of a non-linear generalisation of Onsager's irreversible thermodynamics [Se5]. I shall conclude, in §5, with some further brief comments about the project of a macroscopically-centred statistical mechanics.

2. Macroscopic Quantum Theory of Superconductivity. At the *phenomenological* level, the principal electrodynamic properties of superconductors are their capacity to support persistent electric currents (superconductivity) and their perfect diagmagnetism (Meissner effect). These two properties are intimately related, since the Meissner effect is the mechanism whereby the supercurrents screen the magnetic field they generate from the interior of the body [Lo]. Thus, superconductivity arises from the combination of the Meissner effect with the thermodynamic metastability of the supercurrents and their magnetic fields.

Although it appears to be widely accepted that the microscopic theory of Bardeen-Cooper-Schrieffer [BCS] leads to the electrodynamics of metallic superconductors, the arguments employed both there and in related works [An, Ri] are radically flawed in that (a) they are based on totally uncontrolled approximations, and (b) they violate (exact) gauge covariance of the second kind *at the Hamiltonian level*, and thus do not even admit precise definition of a local current density. As regards ceramic, i.e. high T_c, superconductivity, the microscopic theory is less developed than in the metallic case, and has not yet led to an electrodynamics.

On the other hand, the BCS characterisation of the structure of the superconductive phase by electron pairing, first proposed by Schafroth [Sc], has been amply substantiated by experiments on the Josephson effect [Jo] and the quantisation of trapped magnetic flux in multiply-connected superconductors [DF]. Moreover, Yang [Ya], generalising ideas of O. Penrose [Pe, PO], pointed out that this characterisation is captured by the hypothesis of *off-diagonal long range order* (ODLRO). This is a macroscopic quantum property, representing a well-defined order structure in a gauge covariant way. Furthermore, it is a property also possessed by certain ansätze, e.g. [ZA], for the high T_c superconductive phase of ceramics.

I shall now sketch an approach [Se2,3] I have made to the electrodynamics of superconductors, based on the assumption of ODLRO. This is designed to relate the electromagnetic properties to the order structure of these systems in purely macroscopic quantum terms (cf. eqno. (2.8) below). For brevity, I shall confine myself here to the derivation of the Meissner effect from ODLRO.

The Model. We take the quantum model, Σ, to be an infinitely extended system of electrons, and possibly also of ions or phonons, in a Euclidean space X : lattice systems may be formulated analogously. Points in X will generally be denoted by x, (sometimes by y, a or b) and the Lebesgue measure by dx. It will be assumed that the model enjoys the properties of gauge covariance of the second kind, and that its interactions are translationally invariant.

The electronic part of Σ is formulated in terms of a quantised field $\psi = (\psi_\uparrow, \psi_\downarrow)$, satisfying the canonical anticommutation relations. Thus, in a standard way, the $C^\star-$algebra $\mathcal{F}_{el}$ of the CAR over the Hilbert space $\mathcal{H} := L^2(X, dx)$ is defined by the specifictions that

(1) there are linear maps $\psi_\uparrow, \psi_\downarrow$, from $\mathcal{H}$ into $\mathcal{F}_{el}$ satisfying the CAR

$$(2.1) \qquad [\psi_\alpha(f), \psi_\beta(g)^\star]_+ = \delta_{\alpha,\beta}\langle g, f\rangle_{\mathcal{H}}; \; [\psi_\alpha(f), \psi_\beta(g)]_+ = 0$$

(2) $\mathcal{F}_{el}$ is generated by $\{\psi_\alpha(f), \psi_\alpha(f)^\star | f \in \mathcal{H}; \; \alpha = \uparrow, \downarrow\}$.

The algebra $\mathcal{F}_{el}$ is then the *field algebra* of the electrons. Space translations and gauge transformations are represented by the homomorphisms $\sigma_0, \; \gamma$ of the additive groups $X, \; C_R^\infty(X)$, respectively, into $Aut(\mathcal{F}_{el})$, defined by the formulae

$$(2.2) \qquad \sigma_0(a)\psi(f) = \psi(f_a) \; \forall a \in X, \; with \; f_a(x) := f(x - a)$$

and

$$(2.3) \qquad \gamma(\chi)\psi(\phi) = \psi(\phi \exp(i\chi)) \; \forall \chi \in C_R^\infty(X)$$

The *global* gauge automorphisms are those for which χ is constant.

Let $\mathcal{K} := \{f_1 \otimes f_2 | f_1, f_2 \in \mathcal{H}\}$. We define the *pair field* Ψ to be the mapping of $\mathcal{K}$ into $\mathcal{F}_{el}$ given by

$$(2.4) \qquad \Psi(F) = \psi_\uparrow(f_1)\psi_\downarrow(f_2) \; for \; F = f_1 \otimes f_2$$

Hence, by (2.2)-(2.4),

$$(2.5) \qquad \sigma_0(a)\Psi(F) = \Psi(F_a), \; with \; F_a(x_1, x_2) = F(x_1 - a, x_2 - a)$$

and

$$(2.6) \qquad \gamma(\chi)\Psi(F) = \Psi(g(\chi)F);$$

$$with\ (g(\chi)F)(x_1,x_2) := F(x_1,x_2)\exp i(\chi(x_1)+\chi(x_2))$$

In a standard way, we define the *observable algebra* of the electrons to be the subalgebra $\mathcal{A}_{el}$ of $\mathcal{F}_{el}$ that is elementwise invariant under the global gauge automorphisms $\psi\to\psi\exp(i\alpha)$, with α constant. Space translations and gauge transformations of the electronic observables are then given by the restrictions to $\mathcal{A}_{el}$ of the automorphism groups $\sigma_0(X)$ and $\gamma(C_R^{\infty}(X))$, respectively.

The construction of the $C^{\star}-$algebra $\mathcal{A}_0$ of the observables of the other species of particles of Σ is effected in a similar way. We take the $C^{\star}-$algebra of observables of the system to be $\mathcal{A} := \mathcal{A}_{el}\otimes\mathcal{A}_0$ and canonically identify $\mathcal{A}_{el}$ with its subalgebra $\mathcal{A}_{el}\otimes I$. It is assumed that the automorphism groups $\sigma_0(X)$ and $\gamma(C_R^{\infty}(X))$ extend from $\mathcal{A}_{el}$ to $\mathcal{A}$.

We assume, for simplicity,* that the dynamics of Σ, as given by a canonical limiting form of that of finite versions of the system, corresponds to a one-parameter group $\{\alpha(t)|t\in\mathbf{R}\}$ of automorphisms of $\mathcal{A}$.

An equilibrium state ω at inverse temperature β may then be characterised by the Kubo-Martin-Schwinger (KMS) conditions [HHW], namely that, for arbitrary $A,B\in\mathcal{A}$, there is a function F on $\mathbf{C}$ that is analytic in the interior of the strip $Im(z)\in[0,\hbar\beta]$ and continuous on its boundaries, and satisfies the relations

$$F(t)=\omega(A\alpha(t)B);\ F(t+i\hbar\beta)=\omega((\alpha(t)A)B) \tag{2.7}$$

Off-Diagonal Long Range Order. A state ω is said to possess the property of off-diagonal long-range order (ODLRO) if there is a mapping $\Phi:\mathcal{K}\to\mathbf{C}$, such that

$$\lim_{|y|\to\infty}[\omega(\Psi(F)^{\star}\Psi(G_y))-\overline{\Phi(F)}\Phi(G_y)]=0\ \forall F,G\in\mathcal{K} \tag{2.8}$$

where the bar denotes complex conjugation; and $\Phi(G_y)$ does not tend to zero, for all $G\in\mathcal{K}$ as $y\to\infty$.

Φ is then termed the *macroscopic wave function* for the state ω.

Note that, although $\Psi(F)$ does not belong to the observable algebra $\mathcal{A}$, the argument of ω in (2.8) does.

Lemma 2.1. *The ODLRO conditions define the macroscopic wave function up to a constant phase factor; i.e., if Φ_1,Φ_2 are two such functions satisfying these conditions, for the same state ω, then $\Phi_2=\Phi_1\exp(i\eta)$, where η is a real-valued constant.*

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* The more generally valid assumption of a $W^{\star}-$dynamical system [Se6], employed in §4 of this article, leads to precisely the same results as the present one.

Proof. Assuming that Φ_1, Φ_2 both satisfy the ODLRO conditions with respect to the same state ω, it follows from (2.8) that

$$\lim_{|y|\to\infty}[\overline{\Phi_1(F)}\Phi_1(G_y) - \overline{\Phi_2(F)}\Phi_2(G_y)] = 0$$

Since this is valid for all $F, G \in \mathcal{K}$, we may replace F by $F'(\in\mathcal{K})$, thereby obtaining

$$\lim_{|y|\to\infty}[\overline{\Phi_1(F')}\Phi_1(G_y) - \overline{\Phi_2(F')}\Phi_2(G_y)] = 0$$

On multiplying the complex conjugate of the first equation by $\Phi_2(F')$ and that of the second one by $\Phi_2(F)$, and then taking the difference, we see that

$$\lim_{|y|\to\infty}\overline{\Phi_1(G_y)}[\Phi_1(F)\Phi_2(F')) - \Phi_1(F')\Phi_2(F)] = 0 \tag{2.9}$$

Since, by the above definition of ODLRO, there are elements G of $\mathcal{K}$ for which $\Phi(G_y)$ does not tend to zero, as $|y|\to\infty$, it follows that the quantity in the square brackets of (2.9) vanishes. Consequently, as $\Phi_{1,2}$ are non-zero, by the same stipulation,

$$\Phi_2(F) = c\Phi_1(F)\ \forall F \in \mathcal{K}$$

where c is a complex-valued constant, and since Φ_1, Φ_2 both satisfy (2.8), it follows immediately that this is just a constant phase factor $\exp(i\eta)$.

Gauge and Space Translational Covariance. Assume now that the system is subjected to a classical, static magnetic field, of induction

$$B = curl A \tag{2.10}$$

The time-translational automorphisms then become $A-$dependent, and we denote them by $\alpha_A(\mathbf{R})$. We assume that they are covariant w.r.t. space translations and gauge transformations, i.e. that

$$\sigma_0(a)\alpha_A(t)\sigma_0(-a) = \alpha_{A_a}(t);\ with\ A_a(x) := A(x-a) \tag{2.11}$$

and

$$\gamma(\frac{e\chi}{\hbar c})\alpha_A(t)\gamma(\frac{-e\chi}{\hbar c}) = \alpha_{A+\nabla\chi}(t) \tag{2.12}$$

We note now that, in the particular case where B is uniform, it may be represented by the vector potential

$$A = \frac{1}{2}B\times x \tag{2.13}$$

Thus, choosing

$$\chi(x) = -\frac{1}{2}(B\times a).x, \tag{2.14}$$

we see that

$$A + \nabla\chi = A_a \tag{2.15}$$

Hence, defining $\sigma : X \to Aut(\mathcal{A})$ by the formula

$$\sigma(a) = \gamma(\frac{e\chi}{\hbar c})\sigma_0(a), \tag{2.16}$$

it follows from (2.11),(2.12) and (2.16) and the definition of $\mathcal{A}$ that σ is a representation of X in $Aut\mathcal{A}$ which commutes with the time translations $\alpha_A(\mathbf{R})$, with the gauge fixed by equn. (2.13). In view of these properties, we take σ to be the space translational automorphisms in the presence of the uniform magnetic field B.

Note. By (2.5),(2.6) and (2.16), the canonical extension of σ to $\mathcal{F}_{el}$, and in particular to the pair field Ψ, yields

$$\sigma(a)\Psi(F) = \Psi(s(a)F) \tag{2.17}$$

where

$$(s(a)F)(x_1, x_2) = F(x_1 - a, x_2 - a)\exp(\frac{ie(B\times a).(x_1 + x_2)}{2\hbar c}) \tag{2.18}$$

Hence,

$$[s(a), s(b)]_- = 2isin(\frac{eB.(a\times b)}{\hbar c})s(a+b) \ and \ s(a)s(-a) = I \ \forall a, b\in X \tag{2.19}$$

where $[,]_-$ denotes commutator. Thus, as $\sigma(a)$ and $\sigma(b)$ do not, in general intercommute, it follows from (2.17) that the extension of $\sigma(X)$ to the field algebra $\mathcal{F}_{el}$ is non- abelian. This is crucial for our derivation of the Meissner effect below.

ODLRO and the Meissner Effect. The essential distinction between normal diamagnetism and the Meissner effect is that the former can support a uniform, static, non-zero magnetic induction and the latter can not. Thus, we base our derivation of the Meissner effect on considerations of the response of an state with ODLRO to the action of a uniform magnetic field.

Proposition 2.2. *The system cannot support uniform, non-zero magnetic induction in translationally invariant states with ODLRO.*

The following Corollary follows immediately from this Propostion and elementary thermodynamics.

Corollary 2.3. *Assuming that translational symmetry is preserved in the equilibrium state ω_A, then either*

(1) ω_A possesses the property of ODLRO and $B = 0$

or

(2) ω_A does not possess ODLRO and is normally diamagnetic.

Further, assuming that, in the absence of a magnetic field, the free energy density of the ODLRO phase is lower, by Δ, than that of the normal one, the former phase will prevail, and thus the system will exhibit the Meissner effect, provided that the applied field, H, satisfies the condition that $|H| < H_c := (8\pi\Delta)^{1/2}$

Comment. This result signifies that the Meissner effect arises from a rigidity of the macroscopic wave-function in the face of an applied magnetic field. This corresponds precisely to London's [Lo] idea of rigidity, transferred to the macroscopic level.

Proof of Proposition 2.2. By the translational invariance of ω_A and the formula (2.17) for σ,

$$\omega_A(\Psi(s(a)F)^\star\Psi(s(a)G)) \equiv \omega_A(\Psi(F)^\star\Psi(G)) \tag{2.20}$$

Further, it follows from the ODLRO condition (2.8) and the definition (2.18) of s that

$$\lim_{y\to\infty}[\omega_A(\Psi(s(a)F)^\star\Psi(s(a)G_y)) - \overline{\Phi(s(a)F)}\Phi(s(a)G_y)] = 0$$

and hence, by (2.20), that

$$\lim_{y\to\infty}[\omega_A(\Psi(F)^\star\Psi(G_y)) - \overline{\Phi_a(F)}\Phi_a(G_y)] = 0 \tag{2.21}$$

where

$$\Phi_a = \Phi \circ s(a) \tag{2.22}$$

Equation (2.21) implies that Φ_a, as well as Φ, serves as a macroscopic wave function for the state ω_A, and therefore, by Lemma 2.1 and equn. (2.22), that

$$\Phi \circ s(a) = c(a)\Phi$$

where $c(a)$ is a complex number of unit modulus. Similarly, if b is another element of X, then

$$\Phi \circ s(b) = c(b)\Phi$$

where $c(b)$ is also a complex number of unit modulus. Thus, the last two equations imply that

$$\Phi\circ[s(a),s(b)]_- = 0$$

On taking the composition product of this equation with $s(-a-b)$ and using (2.19), we see that,

$$sin(\frac{eB.(a\times b)}{\hbar c})\Phi = 0 \ \forall a, b\in X$$

from which it follows that *either* $B = 0$ *or* $\Phi = 0$, which is the required result.

3. Hydrodynamical Phase Transition in a Quantum Plasma.

The quantum Jellium model is a system of electrons, interacting via Coulomb forces both with one another and with a uniform, positively charged, neutralising background. It is thus a model of a many-particle system with realistic interactions. Its thermodynamic properties have been established at the level of mathematical physics [LN]. I shall now sketch a treatment [Se4,7] leading from its many-particle Schrödinger equation to an Eulerian hydrodynamics with a non-equilibrium phase transition. The three principal stages of the derivation of this result are the following. Firstly, we derive a classical Vlasov equation, governing a *large scale* description of its dynamics, from the microscopic Schrödinger equation, together with certain initial and regularity conditions. Secondly, we observe that the Vlasov dynamics corresponds precisely to the Liouville equation for a *Lagrangian* hydrodynamics, governing the evolution of the time (t)-dependent position, $X_t(x)$, of a 'fluid particle'located initially at the point x. Then, finally, we show that this Lagrangian hydrodynamics reduces to a deterministic *Eulerian* form, provided that a certain parameter, governing the non-uniformity in the initial density profile, lies below a certain critical value, and that otherwise it corresponds to a *stochastic* flow.

The Jellium Model, $\Sigma^{(N,L)}$, consists of N electrons in a cube, $K^{(L)}$, of side L, with uniform neutralising positive charge background. We assume periodic boundary conditions. Our objective is to obtain a quantum theoretical derivation of the hydrodynamics of $\Sigma^{(N,L)}$ in a limit where N and L tend to infinity and the mean particle density,

$$\overline{n} = N/L^3 \tag{3.1}$$

remains fixed and finite.

Denoting the gradient operator in $K^{(L)}$ by $\nabla^{(L)}$, we represent the position vectors and momenta of the electrons by the standard multiplicative and differential operators $\{X_j, P_j = -i\hbar\nabla_j^{(L)} | j = 1, .. N\}$ in the Hilbert space $\mathcal{H}^{(N,L)}$ of square integrable antisymmetric functions on $(K^{(L)})^N$. The Hamiltonian is then the self-adjoint operator in $\mathcal{H}^{(N,L)}$ given by

$$H^{(N,L)} = \frac{-\hbar^2}{2m}\sum\nolimits_{j=1}^{N} \Delta_j^{(L)} + e^2 \sum\nolimits_{j,k(>j)=1}^{N} U^{(L)}(X_j - X_k) \tag{3.2}$$

where $-e, m$ are the electronic charge and mass, respectively, $\Delta^{(L)}$ is the Laplacian for $K^{(L)}$, and $U^{(L)}(X)$ is the difference between $|X|^{-1}$, periodicised w.r.t. $K^{(L)}$, and its space average over that cube, i.e.

$$U^{(L)}(X) = \frac{4\pi}{L^3} \sum\nolimits^{(L)} \frac{\exp(iQ.X)}{Q^2} \tag{3.3}$$

the superscript (L) over Σ signifying that summation is taken over the non-zero vectors $Q = (2\pi/L)(n_1, n_2, n_3)$, with the n's integers. The pure states of $\Sigma^{(N,L)}$ are represented by the normalised vectors, $\Psi^{(N)}$ in $\mathcal{H}^{(N,L)}$ and their evolution is governed by the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi_T^{(N)}}{\partial T} = H^{(N,L)} \Psi_T^{(N)} \tag{3.4}$$

with T the time variable. We shall assume the following initial kinetic and potential energy bounds for $\Sigma^{(N,L)}$-more precisely, for the family of systems $\{\Sigma^{(N,L)}\}$, with N, L satisfying (3.1).

$(I.1)^{(L)}$ The expectation value of the total kinetic energy per particle, for the initial state $\Psi_0^{(N)}$, is less than some finite $N-$independent constant $B/2m$, i.e.

$$(\Psi_0^{(N)}, P_1^2 \Psi_0^{(N)}) < B \tag{3.5}$$

$(I.2)^{(L)}$ The expectation value of the total potential energy, for the the initial state $\Psi_0^{(N)}$, is less than some finite $N-$independent constant, $e^2C/2$, times $N^{5/3}$. This bound corresponds to the electrostatic energy of a continuous distribution of charge, whose density is a smooth function of X/L, and signifies that

$$(\Psi_0^{(N)}, U^{(L)}(X_1 - X_2) \Psi_0^{(N)}) < CN^{2/3} \tag{3.6}$$

We base our macroscopic description of the model on scales of length, time and particle momentum given by L, ω^{-1} and $mL\omega$, where ω is the classical plasma frequency, i.e.

$$\omega = (4\pi\overline{n}e^2/m)^{1/2} \tag{3.7}$$

For this description, we employ the rescaled space and time coordinates, $x = X/L$, $t = \omega T$, respectively. Under this rescaling, $\Sigma^{(N,L)}$ is mapped onto a system $\Sigma^{(N)}$ of particles in a unit cube, K, with periodic boundaries. This rescaling induces a unitary mapping of $\mathcal{H}^{(N,L)}$ onto the Hilbert space $\mathcal{H}^{(N)}$ of antisymmetric square integrable functions on K^N, under which $\Psi_T^{(N)}$ is transformed to the state of $\Sigma^{(N)}$ given by

$$\psi_t^{(N)}(x_1, \ldots, x_N) = L^{3N/2}\Psi_{\omega^{-1}t}^{(N)}(Lx_1, \ldots, Lx_N) \tag{3.8}$$

The Schrödinger equation (3.4) thus transforms to

$$i\hbar_N \frac{\partial \psi_t^{(N)}}{\partial t} = H^{(N)}\psi_t^{(N)} \tag{3.9}$$

where

$$H^{(N)} = \frac{1}{2}\sum_{j=1}^{N} p_j^2 \; + \; N^{-1}\sum_{j,k(>j)=1}^{N} U(x_j - x_k) \tag{3.10}$$

$$p_j = -i\hbar_N \nabla_j \tag{3.11}$$

$$\hbar_N = \frac{\hbar}{mL^2\omega} = \frac{\hbar}{m\omega}(\frac{\overline{n}}{N})^{2/3} \tag{3.12}$$

is a dimensionless effective 'Planck constant', ∇ is the gradient operator for K, and

$$U(x) = \sum_q^{(1)} \exp(iq.x)/q^2 \tag{3.13}$$

the superscript (1) over Σ signifying that summation is taken over the non-zero vectors $2\pi(n_1, n_2, n_3)$, with the n's integers. It follows from (2.13) that

$$\Delta U(x) = 1 - \delta(x) \tag{3.14}$$

where Δ is the Laplacian and δ the Dirac distribution for K.

We formulate the dynamics of $\Sigma^{(N)}$ in terms of its characteristic functions

$$\mu_t^{(N,n)}(\xi_1, \ldots, \xi_n; \eta_1, \ldots, \eta_n) := \tag{3.15}$$

$$(\psi_t^{(N)}, \Pi_{j=1}^{n}(\exp(i\xi_j.p_j/2)\exp(i\eta_j.x_j)\exp(i\xi_j.p_j/2))\psi_t^{(N)})$$

where the ξ's and η's run over the ranges $\mathbf{R}^3$ and $(2\pi\mathbf{Z})^3$, respectively.

The initial condition for $\Sigma^{(N)}$, corresponding to $(I.1)^{(L)}$ for $\Sigma^{(N,L)}$, is

$(I.1)$

$$(3.16) \qquad (\psi_0^{(N)}, p_1^2\psi_0^{(N)}) < N^{-2/3}b \to 0 \ as \ N\to\infty$$

where b is a finite constant.

The initial condition $(II.2)^{(L)}$ transforms to the following form for $\Sigma^{(N)}$, which is unaffected by the above rephasing of the initial state.

$(I.2)$

$$(3.17) \qquad (\psi_0^{(N)}, U(x_1 - x_2)\psi_0^{(N)}) < c$$

where c is a finite constant. We further assume that

$(I.3)$

$$(3.18) \qquad \lim_{N\to\infty}\rho_0^{(N,1)}(x) = \sigma_0(x) \ \forall x \in K$$

where the function σ_0 is continuous; and that

$(I.4)$

$$(3.19) \qquad \lim_{N\to\infty}(\mu_0^{(N,n)}(\xi_1, .\,.\,., \xi_n; \eta_1, .\,.\,., \eta_n) - \Pi_1^n \mu_0^{(N,1)}(\xi_j, \eta_j)) \equiv 0$$

This last condition signifies that, in the limit $N\to\infty$, the initial correlations of $\Sigma^{(N)}$ are of zero range: the assumption behind this is that the initial state of the microscopic model $\Sigma^{(N,L)}$, carries only short range correlations, as in a pure phase [Ru, Se1].

We note here that it was shown by explicit construction, in the Appendix of Ref. [Se7], that the initial conditions (I.1)-(I.4) are perfectly viable.

The macroscopic dynamics of the Jellium model, then, is represented by the time-dependence of the characteristic functions $\mu_t^{(N,n)}$, in the limit $N\to\infty$, subject to the initial conditions (I.1-4).

The Vlasov Dynamics. We note now that the dynamics of the model $\Sigma^{(N)}$, as given by (3.9) and (3.10), has the simplifying features that (a) the effective, dimensionless Planck constant, $\hbar_N$, governing its quantum behaviour, tends to zero as $N\to\infty$; and (b) the pair interaction potential scales as N^{-1}. The properties (a) and (b) are generally the hallmarks of a classical and of a mean field theory, respectively, in the limit $N\to\infty$. In fact, were it not for the Coulomb singularity in U, on e could infer immediately from [NS, Sp] that the Schrödinger equation (3.9), subject to the initial conditions (I.1-4), led to a classical (mean field theoretic) Vlasov dynamics in the limit $N \to \infty$. Specifically, if the two-body potential U in (3.10) were a twice continuously differentiable function, then the following results would prevail.

(A) [NS, Sp] Pointwise convergence of $\mu_t^{(N,1)}$, as $N \to \infty$, to the characteristic function, μ_t, of a classical probability measure m_t on $(K \times \mathbf{R}^3)$, that satisfies the weak Vlasov equation

$$\frac{d}{dt}\int f(x,v)dm_t(x,v) = \int v.\frac{\partial}{\partial x}f(x,v)dm_t(x,v) \tag{3.20}$$

$$-\int \nabla U(x-y).\frac{\partial}{\partial v}f(x,v)dm_t(x,v)dm_t(y,w) \ \forall f \in C_0^2(K \times \mathbf{R}^3)$$

(B) [NS, Sp] Pointwise convergence of $\mu_t^{(N,n)}$ to the characteristic function of the classical probability measure $m_t \otimes m_t .. . \otimes m_t$ $(n \ factors)$ on $(K \times \mathbf{R}^3)^n$.

(C) [Se7] The initial condition for m, ensuing from (I.1) and (I.3), that

$$\int dm_0(x,v)f(x,v) = \int dx\sigma_0(x)f(x,0) \tag{3.21}$$

(D)[Ne, Se7] The unique determination of the solution of the Vlasov equation (3.20), subject to the initial condition (3.21), by that of the Newtonian mean field theoretic problem

$$\frac{dX_t(x)}{dt} = V_t(x); \ \frac{dV_t(x)}{dt} = -\int dy\sigma_0(y)\nabla U'(X_t(x) - X_t(y)); \tag{3.22}$$

$$with \ X_0(x) = x; \ V_0(x) = 0$$

according to the formula

$$\int dm_t(x,v)f(x,v) = \int dx\sigma_0(x)f(X_t(x), V_t(x)) \tag{3.23}$$

In order to extend these results to the Jellium model, $\Sigma^{(N)}$, we require certain regularity conditions on the dynamics of the system, that serve to tame the Coulomb singularity. Accordingly, we invoke certain supplementary assumptions (R), specified in [Se4], whose essential import is that the Coulomb repulsion keeps the electrons apart, sufficiently to ensure that the magnitude of the internal electric field remains bounded. Under these assumptions, we have the following result.

Proposition 3.1.[Se4] *The Schrödinger equation (3.10) for* $\Sigma^{(N)}$, *together with the initial conditions (I.1-4) and the regularity conditions R, leads to the Vlasov dynamics specified by (A)-(D).*

Eulerian Versus Stochastic Hydrodynamics. The Newtonian mean field theory, given by (3.22), corresponds to a *Lagrangian* hydrodynamics, in which $X_t(x)$ and $V_t(x)$ are the position and velocity, respectively, of a 'fluid particle'; and the Vlasov equation (3.20) is just the Liouville equation representing its probabilistic description. Our aim now is to show that the reducibility of the Vlasov dynamics to a deterministic Eulerian hydrodynamics depends on the invertibility of X_t.

Case (a): X_t Invertible. In this case, the Jacobean

$$J_t(x) = \frac{\partial(X_t^{(1)}, X_t^{(2)}, X_t^{(3)})}{\partial(x^{(1)}, x^{(2)}, x^{(3)})} \tag{3.24}$$

with $x^{(j)}$ (resp. $X_t^{(j)}$) the j'th component x (resp. X_t), is strictly positive, and so we can define

$$\sigma_t(x) = \sigma_0(X_t^{-1}(x))/J_t(x);\ \textit{and}\ u_t(x) = V_t(X_t^{-1}(x)) \tag{3.25}$$

Thus, since, by (3.23) and (3.25),

$$\int dm_t(x,v)f(x,v) = \int dx\sigma_t(x)f(x,u_t(x))\ \forall f\in C(K) \tag{3.26}$$

i.e., formally,

$$dm_t(x,v) = \sigma_t(x)\delta(v - u_t(x))dxdv$$

it follows that $u_t(x)$ and $\sigma_t(x)$ are the drift velocity and normalised particle density, respectively, at position x and time t. Moreover, by (3.14), (3.22) and (3.25), u_t, σ_t evolve according to the Euler-cum-Maxwell hydrodynamical equations

$$\frac{\partial\sigma_t}{\partial t} + \nabla.(\sigma_t u_t) = 0;\ \frac{\partial u_t}{\partial t} + (u_t.\nabla)u_t = E_t;\ \nabla.E_t = (\sigma_t - 1) \tag{3.27}$$

Case (b): X_t Non-Invertible. In this case, we cannot employ the formulae (3.25) to define the time-dependent density and drift velocity. Instead, we have to consider the situation where the equation

$$X_t(y) = x$$

has several solutions, labelled by an index set S, for y as a function of x and t, i.e.

$$y = \{Y_t^{(s)}(x)|s\in S\}$$

In this case, equation (3.26) implies that

$$\int dm_t(x,v)f(x,v) = \sum\nolimits_{s\in S}\int dx\sigma_t^{(s)}(x)f(x,u_t^{(s)}(x)) \tag{3.28}$$

where

$$\sigma_t^{(s)}(x) = \sigma_0(Y_t^{(s)}(x))|K_t^{(s)}(x)|; \quad u_t^{(s)}(x) = V_t(Y_t^{(s)}(x)) \tag{3.29}$$

and

$$K_t^{(s)}(x) = \frac{\partial(Y_t^{(s,1)}, Y_t^{(s,2)}), Y_t^{(s,3)})}{\partial(x^{(1)}, x^{(2)}, x^{(3)})} \tag{3.30}$$

Thus, (3.28) signifies that the macroscopic state of the system at time t corresponds to a statistical mixture of different streams, indexed by S, with dnsities $\sigma_t^{(s)}$ and drift velocities $u_t^{(s)}$. This implies that the local density and drift velocity of the system are now *stochastic* variables of a hydrodynamics still governed by the Vlasov equation.

We may summarise the above observations in the following form.

Proposition 3.2. *If X_t is invertible, then the macroscopic dynamics of the system corresponds to a deterministic hydrodynamics given by the Euler-cum-Maxwell equations (3.27). Otherwise, it is a stochastic flow, still governed by the Vlasov equation.*

Example of Hydrodynamic Phase Transition. Let us now specialise to the situation where σ_0 is a function of just a single coordinate, $x^{(1)}$. In this case, as the regularity conditions (R) imply uniqueness of the solution of (3.22) [Se4], the flow becomes effectively one-dimensional, with $X_{1,t}$ dependent on the coordinate $x^{(1)}$ only, and $X_t^{(2)}, X_t^{(3)}$ remaining fixed at $x^{(2)}, x^{(3)}$, respectively. For notational convenience, we shall henceforth drop the superscript (1) from $X_t^{(1)}$ and $x^{(1)}$, and denote by $X_t(x)$ the first component of the vector hitherto represented by this symbol. Thus, by equations (3.22),

$$X_t(x) = x + \int_0^t ds(t-s)\int_0^1 dy\sigma_0(y)F(X_s(x) - X_s(y)) \tag{3.31}$$

where

$$F(x) = -\int_0^1 dx^{(2)}\int_0^1 dx^{(3)}\frac{\partial U}{\partial x}(x, x^{(2)}, x^{(3)}) \tag{3.32}$$

Let

$$J_t(x) = \frac{\partial X_t(x)}{\partial x} \tag{3.33}$$

Then, by Prop. 3.2 and the implicit function theorem, the neccessary and sufficient condition for deterministic hydrodynamics is that J_t has no zeroes.

We note also that the definition (3.33) permits us to re-express (3.31) in the form

$$(3.31)' \qquad X_t(x) = x + \int_0^t ds(t-s)\int_0^1 dy\sigma_0(y)F(\int_y^x dzJ_s(z)))$$

Proposition 3.3. *Under the specified assumptions, the hydrodynamics of the model is deterministic and given by the Euler-cum-Maxwell equations (3.27), provided that*

$$(3.34) \qquad \sigma_0(x) > \frac{1}{2}\forall x\in[0,1]$$

Otherwise there is a transition to a stochastic flow at a certain time τ, given by the least positive value of t for which

$$(3.35) \qquad \sigma_0(x) + (1-\sigma_0(x))\cos(t) = 0$$

for some $x\in[0,1]$.

Proof. By (3.13), (3.14) and (3.31)-(3.33),

$$(3.36) \quad J_t(x) = 1 + \int_0^t ds(t-s)J_s(x)(-1 + \int_0^1 dy\sigma_0(y)\delta(X_s(x) - X_s(y)))$$

where now δ is the Dirac distribution on $[0,1]$, subject to periodic boundary conditions.

Let us first suppose that X_t is invertible, i.e. that J_t is strictly positive, over a time interval $0\leq t < \tau_0$, for some positive τ_0. In this case,

$$J_s(x)\delta(X_s(x) - X_s(y))\equiv\delta(x-y) \ \forall s\in[0,\tau_0)$$

and therefore (3.36) reduces to

$$J_t(x) = 1 + \int_0^t ds(t-s)(\sigma_0(x) - J_s(x))$$

i.e.

$$(\frac{d^2}{dt^2} + 1)J_t(x) = \sigma_0(x); \ \ with \ J_0(x) = 1; \ \dot{J}_0(x) = 0$$

where $\dot{J}_t = dJ_t/dt$. Hence,

$$J_t(x) = \sigma_0(x) + (1-\sigma_0(x))\cos(t)$$

In view of the non-negativity of σ_0, this equation implies that J_t is strictly positive for all $t\geq 0$ if and only if the condition (3.34) is fulfilled. Otherwise,

J_t changes sign at some point $x \in [0,1]$ when t reaches the value τ specified in the statement of the Proposition. Hence, our assumption of the invertibility of X_t is untenable if (3.34) is violated; and therefore, by Prop. 3.2, the flow becomes stochastic in this case.

The proof (cf. [Se4]) of the converse, i.e. that (3.34) implies the invertibility of X_t and thus the deterministic Euler- cum-Maxwell flow, stems from the explicit form of our regularity condition (R).

4. Macrostatistics and Non-Equilibrium Thermodynamics. Here, I present an approach to the general problem of formulating the structures imposed on non-equilibrium thermodynamics by the underlying quantum mechanics of many-particle systems. This is based on a combination of macroscopic and microscopic treatments of a generic system, Σ, of particles occupying a Euclidean space $X = \mathbf{R}^d$. The argument consists of four parts. The first (§4.1) is a formulation of a mathematical framework for non-equilibrium thermodynamics, based on a macroscopic, continuum mechanical model, M, of Σ. The second (§4.2) is an algebraic quantum statistical formulation of a microscopic model, $\mathcal{Q}$ of the same system. The third (§4.3) consists of a treatment of the connection between M and $\mathcal{Q}$, leading to a *classical macrostatistical mechanics* ($CMSM$) of the observables of $\mathcal{Q}$ that correspond to the hydrodynamical variables of M. This admits a clear formulation of *local equilibrium* conditions and of a generalised version of Onsager's regression hypothesis [On], namely that the macroscopic fluctuations about the flow given by M is governed by the same dynamics as the externally induced 'weak' perturbations to that flow. In §4.4, I derive a generalised form of the Onsager reciprocity relations for M from the structure of $CMSM$. The key elements of this derivation are the symmetry properties of the model, stemming from the microscopic reversibility of $\mathcal{Q}$, and the assumption of local equilibrium.

4.1. The Macroscopic Model, M. In the classical thermodynamical description, the *equilibrium states* of Σ are represented by a certain set $q = (q_1, .. ., q_n)$ of intensive variables, corresponding to global densities of extensive conserved quantities, which we shall characterise in §4.2. Its entropy density, s, is then a function of these variables, and its equilibrium properties of governed by the form of s. The thermodynamic variables $\theta = (\theta_1, .. ., \theta_n)$ conjugate to q are defined by the formula

$$\theta = \frac{\partial s(q)}{\partial q}, \ i.e. \ \theta_k = \frac{\partial s(q)}{\partial q_k}, \ k = 1, 2.. , n \tag{4.1}$$

and the pressure, p, is the function of θ given by

$$p(\theta) = sup_q (s(q) - q.\theta) \tag{4.2}$$

the dot representing the $\mathbf{R}^n$ inner product. Thus, the inverse of the formula (4.1) (in the pure phase region) is

$$q = -\frac{\partial p(\theta)}{\partial \theta} \tag{4.3}$$

In non-equilibrium thermodynamics, the state of the system is generally not translationally invariant, and the macroscopic variables q become functions of position, x, and of time, t. In other words, the macrostate is an n-component *classical field*

$$q(x,t) \equiv q_t(x) \equiv (q_{1,t}(x), .. ., q_{n,t}(x)).$$

The laws of continuum mechanics, such as those of hydrodynamics or heat conduction, are then of the *deterministic* form

$$\dot{q}_t = \mathcal{F}(q_t) \tag{4.4}$$

where $\mathcal{F}$ is some functional of the fields q_t. Equivalently, defining the local thermodynamic conjugates θ_t of the fields q_t by

$$\theta_t(x) \equiv \theta(x,t) := \frac{\partial s(q(x,t))}{\partial q}, \tag{4.5}$$

it follows from (4.3) that the equation of motion (4.4) may be re-expressed as

$$\dot{q}_t \equiv \frac{d\dot{q}_t}{dt} = \Phi(\theta_t);\ \Phi := \mathcal{F} \circ (-\frac{\partial p}{\partial \theta}) \tag{4.6}$$

Note. The definition (4.5) of θ_t does not require the microstate of Σ to simulate one of equilibrium at a local level. On the other hand, some assumption of local equilibrium will be needed for the determination of properties of the functional $\mathcal{F}$.

Example. An example of a law of the above form is the non- linear, n-component diffusion given by

$$\dot{q}_{k,t} = \sum_{l=1}^{n} \nabla.(L_{k,l}(\theta_t)\nabla\theta_{l,t}) \tag{4.6a}$$

Returning to the general structure, we impose the following assumptions on the dynamical law (4.6).

(M.1) *The system is confined to a single phase region, i.e. the values of* $q_t(x),\ \theta_t(x)$ *always lie in domains where the functions* s *and* p *are* $C^{(\infty)}$.

(M.2) $\mathcal{F}(q)=0$ *if* $q(x)$ *is constant, i.e. the system is in equilibrium if its local thermodynamic variables* $q(x)$ *(or equivalently* $\theta(x)$*) are spatially uniform.*

(M.3) *The equation of motion (4.6) is covariant w.r.t. space-time translations and scale transformations* $x\to\lambda x, t\to\lambda^r t$, *with* r *a positive integer (=2 in the case of (4.6a)).**

Let $y_t,\ \eta_t$ be 'small' perturbations of $q_t,\ \theta_t$, respectively, and let

$$[\Lambda(\theta)\eta_t](x) := \frac{d}{dz}\Phi(\theta_t(x)+z\eta_t(x))|_{z=0} \tag{4.7}$$

in the pointwise sense, for the class of functions η_t for which the r.h.s. of this formula is well-defined. Then it follows from (4.6) and (4.7) that the *linearised* equation of motion for y_t is

$$\dot{y}_t = \mathcal{L}(\theta_t)y_t \tag{4.8}$$

where

$$\mathcal{L}(\theta_t) = \Lambda(\theta_t)B(\theta_t) \tag{4.9}$$

and $B(\theta)$ is the Hessian $s''(q)$, i.e.

$$(B(\theta))y)_k := \sum\nolimits_{l=1}^{n}\frac{\partial^2 s(q)}{\partial q_k \partial q_l}y_l \tag{4.10}$$

The next assumption permits us to formulate the perturbed dynamics as the evolution of a tempered distribution. Thus, defining $\mathcal{S}^{(n)}(X)$ to be the space of the Schwartz $\mathcal{S}-$class $\mathbf{R}^n-$ valued functions on X, and $\mathcal{S}^{(n)\prime}(X)$ to be its dual space, we assume that

(M.4) *the linear operator* $\mathcal{L}(\theta_t)$ *extends, by continuity, to a transformation of* $\mathcal{S}^{(n)\prime}(X)$, *and the formula (4.8), considered now as an equation of motion in that space, has a unique solution*

$$y_t = T(\theta_.|t,t')y_{t'}\ \forall t\geq t'\geq 0 \tag{4.11}$$

with

$$T(\theta_.|t,t_0)\equiv T(\theta_.|t,t_1)T(\theta_.|t_1,t_0) \textit{ and } T(\theta_.|t,t)=1\ \forall t\geq t_1\geq t_0\geq 0$$

---

* Note that this assumption is not always fulfilled: for example, the Navier-Stokes equation is not scale invariant.

Comments. In the equilibrium case, where $\theta_t = \overline{\theta}$, a constant, the two-parameter family $T(\theta|,.,)$ of transformations of $\mathcal{S}^{(n)\prime(X)}$ reduces to a one-parameter semi-group $\{\tilde{T}(\overline{\theta}|t)|t\in\mathbf{R}_+\}$, where

$$\tilde{T}(\overline{\theta}|(t-t_0)\equiv T(\overline{\theta}|(t,t_0) = \exp(\mathcal{L}(\overline{\theta})(t-t_0)) \tag{4.12}$$

Further, in the case of the non-linear diffusion (4.6a), $\mathcal{L}(\theta^{(0)})$ reduces to the form

$$\mathcal{L}(\overline{\theta}) = L(\overline{\theta})B(\overline{\theta})\Delta;\ L(\overline{\theta}) = [L_{kl}(\overline{\theta})];\ B = [B_{kl}(\overline{\theta})] \tag{4.12a}$$

where Δ is the Laplacian.

The following Proposition follows immediately from (M.1) and (M.4).

Proposition 4.1. *The process $y.$ is covariant w.r.t. space translations and space-time scale transformations, i.e. defining*

$$\phi_t^{(a,b,\lambda)}(x)\equiv\phi^{(a,b,\lambda)}(x,t) := \phi(a+\lambda x, b+\lambda^r t),\ for\ \phi = \theta, q, y \tag{4.13}$$

and for arbitrary $(a,b,\lambda)\in X\times\mathbf{R}\times\mathbf{R}_+)$,

$$(T(\theta_.|t,t')y_{t'})^{(a,b,\lambda)}\equiv T(\theta_.^{(a,b,\lambda)}|t,t')y_{t'}^{(a,b,\lambda)} \tag{4.14}$$

4.2. The Quantum Model, $\mathcal{Q}$. In order to accommodate the dynamics of both the microscopic and macroscopic observables of Σ, we construct its quantum model, $\mathcal{Q}$, as a $W^\star-$dynamical system [Se6] $(\mathcal{A},\alpha,\mathcal{N}(\mathcal{A}))$, where $\mathcal{A}$ is a $W^\star-$algebra of observables, $t\rightarrow\alpha_t$ is a representation of $\mathbf{R}$ in $Aut(\mathcal{A})$, corresponding to the dynamics of the system, and $\mathcal{N}(\mathcal{A}))$ is the folium of normal states on $\mathcal{A}$. In fact, this algebra is constructed as the weak closure of the largest locally normal representation, π, of the standard [HHW] quasi-local $C^\star-$algebra, $\tilde{\mathcal{A}}$, that can support the dynamical and thermodynamical structures we require. Thus, we characterise $\mathcal{A},\alpha$ and π according to the following prescription.

(1) Let L be the set of bounded open regions of X. Then for each $\Lambda\in L$, there is a type-I factor, $\mathcal{A}(\Lambda)(\subset\mathcal{A})$, representing the observables of that region and satisfying the conditions of isotony and local commutativity; and $\mathcal{A}$ is the weak closure of $\mathcal{A}_L := U_{\Lambda\in L}\mathcal{A}(\Lambda)$. We extend automorphisms γ of $\mathcal{A}$ to unbounded observables, Q, affiliated* to this algebra, according to the formula

$$\exp(i\lambda\gamma(Q)) = \gamma(\exp(i\lambda Q))\ \forall\lambda\in\mathbf{R} \tag{4.15}$$

* Recall that, if $\mathcal{M}$ is a $W^\star-$algebra of operators in a Hilbert space $\mathcal{H}$, then the unbounded operators, in $\mathcal{H}$, affiliated to $\mathcal{M}$ are the densely defined ones that commute with $\mathcal{M}'$.

We similarly extend anti-automorphisms of $\mathcal{A}$ to its unbounded affiliates.

(2) The local energy observable (Hamiltonian) $H(\Lambda)$ for the region $\Lambda(\in L)$ is, in general, an unbounded one, affiliated to $\mathcal{A}(\Lambda)$. We assume that $\mathcal{A}$ is equipped with a Wigner time-reversal anti-automorphism, ρ, which leaves this observable invariant, i.e.

$$\rho H(\Lambda) = H(\Lambda) \tag{4.16}$$

(3) Space translations are represented by a homomorphism σ of X into $Aut(\mathcal{A})$, such that $\sigma(x)\mathcal{A}_0(\Lambda)\equiv\mathcal{A}_0(\Lambda+x)$ and $\sigma(x)H(\Lambda) = H(\Lambda+x)$), this last condition representing an assumption of translationally invariant interactions.

(4) The dynamical automorphisms α are given by infinite volume limits of those of finite versions of Σ, according to the formula

$$\alpha_t A = s - \lim_{\Lambda\uparrow}(\exp(iH(\Lambda)t/\hbar)A\exp(-iH(\Lambda)t/\hbar)) \ \forall t\in\mathbf{R},\ A\in\mathcal{A}_L \tag{4.17}$$

Thus, by the translational covariance of $H(\Lambda)$, α_t commutes with the space translational automorphisms, σ, and, by (4.16), satisfies the *microscopic reversibiliy* condition

$$\rho\alpha_t\rho = \alpha_{-t} \ \forall t\in\mathbf{R} \tag{4.18}$$

(5) We formulate the thermodynamics of the system in terms a Hermitian quantum field $\hat{q} = (\hat{q}_1, ..., \hat{q}_n)$, the $\hat{q}_k's$ being densities of locally conserved quantities. We assume that $\hat{q}$ is a tempered distribution, affiliated to $\mathcal{A}$, that transforms covariantly w.r.t space translations. Thus, $\hat{q}$ is a mapping of $\mathcal{S}^{(n)}(X)$ into the self-adjoint affiliates of $\mathcal{A}$. We assume that the function $\exp(i\hat{q}(.))$ is strongly continuous, and that $\hat{q}$ transforms covariantly w.r.t. space translations, i.e.

$$\sigma(x)[\hat{q}(f)] = \hat{q}(f_x),\ where\ f_x(y) = f(x-y)\ \forall x, y\in X, f\in\mathcal{S}^{(n)}(X) \tag{4.19}$$

We assume, for simplicity, that $\hat{q}$ is invariant under time reversals, i.e.

$$\rho\hat{q}(f)\equiv\hat{q}(f) \tag{4.20}$$

and that its components satisfy the following commutation relations, which signify that their space integrals over finite volumes intercommute, up to 'surface effects'.

$$[\hat{q}_k(g), q_l(h)]_- = i\hbar j_{k,l}(\nabla(gh)) \ \forall g, h\in\mathcal{S}(X), \tag{4.21}$$

where $(gh)(x) := g(x)h(x)$ and $j_{k,l}$ a tempered distribution. Further, denoting $\alpha_t[\hat{q}(f)]$ by $\hat{q}_t(f)$, we assume local conservation law of the form

$$\frac{\partial \hat{q}_t(f)}{\partial t} = j_t(\nabla f) \tag{4.22}$$

where j_t is a tempered distribution.

(6) We take the equilibrium thermodynamic variables of $\mathcal{Q}$ to be the 'observables at infinity' [LR], given by the global spatial average $\hat{q}^{\infty}$ of $\hat{q}$ over X. Further, denoting by $\hat{s}$ the standard [Ru] entropy density functional on the translationally invariant states on $\mathcal{A}_0$, we assume that these observables form a complete thermodynamic set, in the sense that [Se1, Ch.4]

(a) for each expectation value, q, of $\tilde{q}$, there is precisely one translationally invariant state ($\in \mathcal{N}(\mathcal{A})$) that maximises $\hat{s}$; and

(b) no proper subset of $\hat{q}$ possesses this property.

The equilibrium thermodynamics of the system is thus given by the form of the resultant entropy density, $s(q)$. We identify q, s with the objects denoted by these symbols in the macroscopic model M; and, defining θ according to (4.1), we denote by ω_θ the maximising state of condition (a). We assume that this state is stationary,* i.e. $\alpha-$invariant, in view of the fact that $\hat{q}_\infty$ is a globally conserved quantity; and we designate it as the equilibrium state corresponding to θ, i.e. to q. We note that, by (4.18) and the thermodynamic completeness condition (a),

$$\omega_\theta \circ \rho = \omega_\theta \tag{4.23}$$

(7) We define π to be the largest locally normal representation of $\tilde{\mathcal{A}}$ that supports the dynamical group α and the quantum field $\hat{q}$, as defined above.

Thus, the quantum model, $\mathcal{Q}$, is given by $(\mathcal{A}, \alpha, \sigma, \hat{q}, \mathcal{N}(\mathcal{A}))$, as specified by the conditions (1)-(7).

4.3. Relationship between M and $\mathcal{Q}$. Our formulation of this relationship is based on the idea that the phenomenological law (4.6) corresponds to the dynamics of the quantum field $\hat{q}$ in a large-scale limit. Thus, in view of the scale-invariance assumption (M.1) for M, we introduce a length parameter L and reformulate $\mathcal{Q}$ on a length scale L and a time scale L^r, defining the quantum field $\hat{q}^{(L)}$ on these scales by the formula

$$\hat{q}_t^{(L)}(f) \equiv \hat{q}^{(L)}(f, t) := \hat{q}(f^{(L)}, L^r t) \tag{4.24}$$

* The proof of this is straightforward for lattice systems, since one can show within the framework of [Se1,Ch.4], that, for these, ω_θ satisfies the KMS conditions, and is therefore stationary.

where

$$f^{(L)}(x) := L^{-d} f(x/L) \tag{4.25}$$

We assume that L is also the length scale of spatial variations of the initial state, $\omega^{(L)}$, of $\mathcal{Q}$, i.e. that there is a map $A \to \overline{A}$ of $\mathcal{A}$ into $C(X)$ and a tempered distribution $q_0 (\in \mathcal{S}^{(n)\prime})$, such that

$$\lim_{L\to\infty} \omega^{(L)}(\sigma(Lx)[A]) = \overline{A}(x) \ \forall x \in X \tag{4.26}$$

and

$$\lim_{L\to\infty} \omega^{(L)}(\hat{q}_0^{(L)}(f)) = q_0(f) \ \forall f \in \mathcal{S}^{(n)} \tag{4.27}$$

We define the fluctuation field $\hat{\xi}^{(L)}$ by the formula

$$\hat{\xi}_t^{(L)}(f) := L^{d/2}(\hat{q}_t^{(L)}(f) - \omega^{(L)}(\hat{q}_t^{(L)}(f))), \ \forall f \in \mathcal{S}^{(n)}(X), \ t \in \mathbf{R} \tag{4.28}$$

Our basic assumptions for the large-scale dynamics of the model are the following.

(I) *For each $M-$ process $q_.$, there is an equivalence class of initial states, $\{\omega^{(L)}\}$, parametrised by L, such that*

(a) the mapping

$$f^{(1)}, .. ., f^{(m)}; t^{(1)}, . ., t^{(m)} \to \omega^{(L)}(\hat{\xi}_{t^{(1)}}^{(L)}(f^{(1)}) .. .(\hat{\xi}_{t^{(m)}}^{(L)}(f^{(m)}))$$

of $(\mathcal{S}^{(n)})^m \times \mathbf{R}^m)$ into $\mathbf{C}$ is continuous, for all positive integers m.

(b) The expectation value of the quantum field $\hat{q}_t^{(L)}$ reduces to that of the classical one, q_t, of M in the limit $L \to \infty$, i.e.

$$\lim_{L\to\infty} \omega^{(L)}(\hat{q}_t^{(L)}(f))) = q_t(f) \ \forall f \in \mathcal{S}^{(n)}(X) \tag{4.29}$$

where q_t is the solution of (4.4), with initial value given by (4.27).

(c) The quantum stochastic process $\hat{\xi}^{(L)}$ converges to a classical one, ξ, as $L \to \infty$, i.e.

$$\lim_{L\to\infty} \omega^{(L)}(\hat{\xi}_{t^{(1)}}^{(L)}(f^{(1)}) .. .(\hat{\xi}_{t^{(m)}}^{(L)}(f^{(m)})) = \tag{4.30}$$

$$\mathbf{E}[\theta_.|(\xi_{t^{(1)}}(f^{(1)}) .. .\xi_{t^{(m)}}(f^{(m)})]$$

$$\forall t^{(1)}, . ., t^{(m)} \in \mathbf{R}_+, \ f^{(1)}, .. ., f^{(m)} \in \mathcal{S}^{(n)}(X), \ r \in \mathbf{N}$$

where the expectation functional $\mathbf{E}[\theta_.|.]$ is governed by the restriction of $\theta_.$ to the close interval between the minimum and maximum of $\{t^{(1)}, . ., t^{(m)}\}$.

Comments. (1) The classicality of the limits of $q^{(L)}$ and $\xi^{(L)}$ here are assumed to arise from the commutation rules (4.21), together with asymptotic abelian properties of $\mathcal{Q}$ with respect to time.

(2) Since (c) implies that the dispersion in $\hat{q}_t^{(L)}$, for the state $\omega^{(L)}$, tends to zero as $L\to\infty$, it follows from (b) that the quantum process $\hat{q}_t^{(L)}$ reduces to the classical one, q_t, in this limit.

(3) It follows from (b) and (c) that ξ_t is an $\mathcal{S}^{(n)\prime}$−valued random variable.

Let

$$\omega_\tau^{(L)} := \omega^{(L)}\circ\alpha(L^r\tau)\ \forall\tau\in\mathbf{R}_+ \tag{4.31}$$

Then $\{\omega_t^{(L)}\}$ satisfies the conditions of (I), and the replacement of $\omega^{(L)}$ by $\omega_\tau^{(L)}$ corresponds to that of $\theta_.$ by $\theta_.^{(\tau)}$ in (4.30), where

$$\theta_t^{(\tau)} = \theta_{t+\tau},\ \forall t,\tau\in\mathbf{R}_+ \tag{4.32}$$

i.e.

$$\mathbf{E}[\theta_.|(\xi_{t^{(1)}+\tau}(f^{(1)})..\ .\xi_{t^{(m)}+\tau}(f^{(m)})]\equiv \tag{4.33}$$

$$\mathbf{E}[\theta_.^{(\tau)}|(\xi_{t^{(1)}}(f^{(1)})..\ .\xi_{t^{(m)}}(f^{(m)})]$$

In the particular case where $t^{(1)} = ..\ = t^{(m)} = 0$, the r.h.s. of this equation depends on $\theta_.^{(\tau)}$ only through the value of $\theta_0^{(\tau)}\equiv\theta_\tau$, by (4.32). Thus, by (4.30), the equal time correlation functions for the process $\xi_.$ are of the form

$$\mathbf{E}[\theta_.|\xi_\tau(f^{(1)})..\ .\xi_\tau(f^{(m)})]\equiv\mathbf{E}[\theta_\tau|\xi_0(f^{(1)})..\ .\xi_0(f^{(m)})] \tag{4.34}$$

Our next assumption is that the space-time clustering properties of $\mathcal{Q}$ render the process $\xi_.$ Gaussian (cf. [GVV]), and that the infinite separation of the relevant relaxation time-scales of the models M and $\mathcal{Q}$ ensure that it is Markovian.

(II) *The process $\xi_.$ is Gaussian and temporally Markovian.*

It follows immediately from this assumption that the process ξ is completely determined by its two-point function. Our next assumption is the following generalisation of Onsager's regression hypothesis [On].

(III) *The fluctuation process ξ is governed by precisely the same dynamics as the perturbation, $y_.$, to the deterministic process $q_.$, i.e., by (4.11),*

$$\mathbf{E}[\theta_.|(\xi_{t+\tau}(f)\xi_t(g)] = \mathbf{E}[\theta_.|(\xi_t(T(\theta_.|t+\tau,t)^\star f)\xi_t(g)]$$

Hence, by (4.34)

$$\mathbf{E}[\theta_{.}|(\xi_{t+\tau}(f)\xi_t(g)] = \mathbf{E}[\theta_t|(\xi_0(T(\theta_t|t+\tau,t)^\star f)\xi_0(g)] \tag{4.35}$$

$$\forall f\in\mathcal{S}^{(n)}(X), t\in\mathbf{R},\ \tau\in\mathbf{R}_+$$

Thus, the process is determined by the form of T and of the expectation functional $\mathbf{E}[\theta_t|.]$ on the algebra generated by ξ_0. In order to formulate the action of space translations and scale transformations on the process, we define

$$f^{(a,\lambda)}(x) := \lambda^{-d/2} f(\lambda^{-1}(x-a))\ \forall a\in X, \lambda\in\mathbf{R}_+ \tag{4.36}$$

and

$$\xi_0^{(a,\lambda)}(f) := \xi_0(f^{(a,\lambda)})\ \forall a\in X, \lambda\in\mathbf{R}_+ \tag{4.37}$$

Proposition 4.2 *Under the above assumptions and definitions,*

$$\mathbf{E}[\theta_b|(\xi_0^{(a,\lambda)}(T(\theta_{.}|b+\tau,b)^\star f)\xi_0^{(a,\lambda)}(g)] = \tag{4.38}$$

$$\mathbf{E}[\theta_0^{(a,b,\lambda)}|\xi_0(T(\theta_{.}^{(a,b,\lambda)}|\tau,0)^\star f)\xi_0(g)]\ \forall a\in X,\ b,\tau\in\mathbf{R}_+,\ \lambda\in\mathbf{R}_+$$

with $\theta_{.}^{(a,b,\lambda)}$ as defined by (4.13).

Proof. The result is obtained by replacing each f by $f^{a\lambda}$, in (4.30), and using equns. (4.13), (4.14), (4.19), (4.27), (4.28), and (4.35)-(4.37).

We note now that the local properties of the process ξ, in the neighbourhood of a space-time point (a,b), is given by the form of the l.h.s. of (4.38), in the limit $\lambda\to 0$. Moreover, by (4.13), the function $\theta_{.}^{(a,b,\lambda)}$, which occurs there, tends pointwise to a constant, $\theta(a,b)$, in this limit. These observations leads us to the following *local equilibrium* assumption.

(V)

$$\lim_{\lambda\to 0}\mathbf{E}[\theta_0^{(a,b,\lambda)}|\xi_0(T(\theta_{.}^{(a,b,\lambda)}|(\tau,0)^\star f)\xi_0(g)] = \tag{4.39}$$

$$\mathbf{E}[\theta(a,b)|(\xi_0(T(\theta(a,b)|\tau,0)^\star f)\xi_0(g)]\ \forall f,g\in\mathcal{S}^{(n)}(X),\ \tau\geq 0$$

and further, the r.h.s. of this formula is precisely the same as for the fluctuations of the field $\hat{q}_{.}$ about an equilibrium state $\omega_{\theta(a,b)}$, as defined in item (6) of §4.2, *i.e.*

$$\mathbf{E}[\theta(a,b)|\xi_0(T(\theta(a,b)|\tau,0)^\star f)\xi_0(g)]\equiv \tag{4.40}$$

$$\lim_{L\to\infty}\omega_{\theta(a,b)}([\alpha(L^r\tau)\hat{\xi}_0(f)]\hat{\xi}_0(g))$$

Hence, by (4.12) and (4.40),

$$\mathbf{E}[\theta(a,b)|\xi_0(\exp(\mathcal{L}(\theta(a,b))\tau))^\star f)\xi_0(g)] = \tag{4.41}$$

$$\lim_{L\to\infty}\omega_{\theta(a,b)}([\alpha(L^r\tau)\hat{\xi}_0(f)]\hat{\xi}_0(g))$$

4.4. Consequences of (I)-(V): Generalised Onsager Relations. Let $\mathcal{R}(\theta)$ be the range of the function $\theta\equiv\{\theta(a,b)|a\in X, b\in\mathbf{R}_+\}$. We shall employ the above theory to obtain properties of $\mathbf{E}[\overline{\theta}|.]$ and $\mathcal{L}(\overline{\theta})$ for arbitrary $\overline{\theta}\in\mathcal{R}(\theta)$.

(a) **Symmetry Property of Time Correlations Functions.** In view of the microscopic reversibility conditions (4.18), (4.20) and (4.23), together with the stationarity of $\omega_{\overline{\theta}}$, it follows from (4.30), with $\omega^{(L)} = \omega_{\overline{\theta}}$, that

$$\omega_{\overline{\theta}}(\xi_t(f)\xi_0(g))\equiv\omega_{\overline{\theta}}(\xi_0(f)\xi_{-t}(g))\equiv\omega_{\overline{\theta}}(\xi_t(g)\xi_0(f))\ \forall\overline{\theta}\in\mathcal{R}(\theta)$$

Hence, by (4.41), we have the symmetry property

$$\mathbf{E}[\overline{\theta}|\xi_0(\exp(\mathcal{L}(\overline{\theta})^\star\tau)f)\xi_0(g)]\equiv\mathbf{E}[\overline{\theta}|\xi_0(\exp(\mathcal{L}(\overline{\theta})^\star\tau)g)\xi_0(f)]\ \forall\overline{\theta}\in\mathcal{R}(\theta) \tag{4.42}$$

(b) **The Static Two-point Function.** It follows immediately from (4.41) that $\mathbf{E}[\overline{\theta}|.]$ inherits the translational invariance of $\omega_{\overline{\theta}}$. Hence, in view of the tempered distribution property of ξ_0, the generalised function $(x,y)(\in X^2)\to\mathbf{E}[\overline{\theta}|(\xi_0(x)\xi_0(y)]$ is an $\mathcal{S}^{(n)\prime}(X)-$ class distribution $F(x-y)$; and, by Prop. 4.2, $F(\lambda x)\equiv\lambda^{-d}F(x)$, and is therefore of the form $C\delta(x)$, where C is an n-by-n matrix. Thus,

$$\mathbf{E}[\overline{\theta}|\xi_0(f)\xi_0(g)] = \langle Cf,g\rangle\ \forall\overline{\theta}\in\mathcal{R}(\theta) \tag{4.43}$$

where the angular brackets denote the inner product for the Hilbert space $\mathcal{H}^{(n)}$ of square integrable functions from X into $\mathbf{R}^n$, as defined by the formula

$$\langle f,g\rangle = \int f(x).g(x)dx \tag{4.44}$$

the dot denoting the $\mathbf{R}^n$ scalar product. Moreover, it follows [Se5] from a treatment of the linear response of $\omega_{\overline{\theta}}$ to local Hamiltonian perturbations $\hat{q}(f)$ that, under mild technical assumptions, $C = B(\theta)^{-1}$, where B is specified in (4.10). Hence, by (4.43),

$$\mathbf{E}[\overline{\theta}|\xi_0(f)\xi_0(g)] = \langle B(\overline{\theta})^{-1}f,g\rangle \tag{4.45}$$

(c) **Generalised Onsager Relations.** It follows immediately from (4.42) and (4.45) that

$$\langle B(\overline{\theta})^{-1}\exp(\mathcal{L}(\overline{\theta})^{\star}\tau)f,g\rangle\equiv\langle B(\overline{\theta})^{-1}\exp(\mathcal{L}(\overline{\theta})^{\star}\tau)g,f\rangle \tag{4.46}$$

Hence, by (4.9), we have the following result.

Proposition 4.3. *Under the above assumptions, Λ satisfies the generalised Onsager relation*

$$\langle\Lambda(\overline{\theta})^{\star}f,g\rangle\equiv\langle\Lambda(\overline{\theta})^{\star}g,f\rangle\ \forall\overline{\theta}\in\mathcal{R}(\theta),\ f,g\in\mathcal{S}^{(n)\prime}(X) \tag{4.47}$$

i.e. $\Lambda(\overline{\theta})$, *considered as an operator in* $\mathcal{H}^{(n)}$, *with domain* $\mathcal{S}^{(n)}$, *is symmetric.*

Comment. In the case of the non-linear diffusion given by (4.6a), it follows from (4.12a) that (4.47) reduces to the form

$$L_{kl}(\theta)(x,t)) = L_{lk}(\theta)(x,t))\ \forall x\in X,\ t\in\mathbf{R}_{+}$$

5. Concluding Remarks. I have endeavoured to show here how, at least in certain domains, a macroscopically-based approach to statistical mechanics can serve to determine the form imposed by quantum mechanics on the structure of phenomenological laws. By contrast with the standard many-body theory, the microscopic imput here is limited to very general principles; and this serves to pare down the conceptual structure of the theory to its essentials.

Of course, the relative simplicity gained by this approach is dependent on a number of assumptions, specified in the previous Sections, that are very difficult to verify constructively. Furthermore, the dynamical systems treated in $\S's$ 3 and 4 have the simplifying, and rather particular, property of scale covariance. In the case of the plasma model, this stems from the fact that the Coulomb potential is given by a power law: in the case of the non-equilibrium thermodynamics of §4, it is an assumed property of the macroscopic dynamics.

Thus, it is clear that the formulation of a coherent, general formulation of the statistical mechanics of macroscopic variables poses deep problems, concerning both its underlying assumptions and its potential scope. I would hope that inroads into these problems may be achieved through the study both of suitable models and of the relevant general structures.

References

[An] P. W. Anderson: Phys. Rev. **110**, 827 (1959)

[BCS] J. Bardeen, L. N. Cooper and J. R. Schrieffer: Phys. Rev. **108**, 1175 (1957)

[DF] B. Deaver and W. M. Fairbank: Phys. Rev. Lett. **7**, 43 (1961)

[GVV] D. Goderis, A. Verbeure and P. Vets: Pp. 178-193 of "Quantum Theory and Applications V", Ed. L. Accardi and W. von Waldenfels, Springer Lecture Notes in Mathematics 1442, 1990

[He] K. Hepp: Helv. Phys. Acta **45**, 237 (1972)

[HL] K. Hepp and E. H. Lieb: Helv. Phys. Acta **46**, 973 (1073)

[HHW] R. Haag, N. M. Hugenholtz and M. Winnink: Commun. Math. Phys. **5**, 215 (1967)

[Jo] B. D. Josephson: Rev. Mod. Phys. **36**, 216 (1964)

[Lo] F. London: Superfluids, Vol. 1, Wiley, London, 1950

[LL] L. D. Landau and I. M. Lifschitz: "Fluid Mechanics", Pergamon Press, Oxford, New York, Paris, 1984

[LN] E. H. Lieb and H. Narnhofer: J. Stat. Phys. **12**, 291 (1975)

[LR] O. E. Lanford and D. Ruelle: Commun. Math. Phys. **13**, 194 (1969)

[Ne] Fluid Dyn. Trans. **9**,229 (1978)

[NS] H. Narnhofer and G. L. Sewell: Commun. Math. Phys. **79**, 9 (1981)

[On] L. Onsager: Phys. Rev. **37**, 405 (1931) and **38**, 2265 (1931)

[Pe] O. Penrose: Phil. Mag. **42**, 1373 (1951)

[PO] O. Penrose and L. Onsager: Phys. Rev. **104**, 576 (1956)

[Ri] G. Rickayzen: Phys. Rev. **115**, 795 (1959)

[Ru] D. Ruelle: "Statistical Mechanics", W. A. Benjamin Inc., New York, 1969 [Sc] M. R. Schafroth: Phys. Rev. **100**, 463 (1955)

[Se1] G. L. Sewell: "Quantum Theory of Collective Phenomena", Oxford University Press, Oxford, 1989

[Se2] G. L. Sewell: J. Stat. Phys. **61**, 415 (1990)

[Se3] G. L. Sewell: "Macroscopic Quantum Theory of Superconductivity and the Higgs Mechanism", to be published in the Proceedings of the 1991 Locarno Conference on "Stochastics, Physics and Geometry".

[Se4] G. L. Sewell: "Quantum Plasma Model with Hydrodynamical Phase Transition", Preprint

[Se5] G. L. Sewell:Pp.77-122 of "Large-Scale Molecular Systems: Quantum and Stochastic Aspects", Nato ASI Series B, Ed. W. Gans, A. Blumen and A. Amann, Plenum, New York and London, 1991

[Se6] G. L. Sewell: Lett. Math. Phys. **6**, 209 (1982)

[Se7] G. L. Sewell: J. Math. Phys. **26**, 2324 (1985)

[Sp] H. Spohn: Math. Meth. Appl. Sci. **3**,445 (1981)

[Ya] C. N. Yang: Rev. Mod. Phys. **34**, 694 1962

[ZA] Z. Zou and P. W. Anderson: Phys. Rev. B **37**, 627 (1987)